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Guilherme Barreto Torres

Decision Making at Early Design Stages: Economic Risk Analysis of Add-On Processes to Existing Sugarcane Biorefineries

TOMADA DE DECISÃO EM FASE INICIAL DE PROJETO: ANÁLISE DO RISCO ECONÔMICO EM ADICIONAR UM PROCESSO NOVO A UMA USINA EXISTENTE

CAMPINAS, 2016

Universidade Estadual de Campinas
Faculdade de Engenharia Química

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A Ata da Defesa, assinada pelos membros da comissão examinadora, consta no processo de vida acadêmica do aluno.

Dedico este trabalho aos meus avós Wilson e Alice.

This work is dedicated to my grandparents: Wilson and Alice.

– That's right! — shouted Vroomfondel, – We demand rigidly defined areas of doubt and uncertainty!

Douglas Adams in The Hitchhiker’s Guide to the Galaxy

– Isso mesmo! — gritou Vroomfondel, – Exigimos áreas de dúvida e incerteza rigidamente delimitadas!

Douglas Adams em O Guia do Mochileiro das Galáxias

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Resumo

Em fases iniciais de projetos de plantas químicas, são estudados aspectos dos processos que são definidos, em muitos casos, de acordo com o conhecimento e as experiências passadas das pessoas envolvidas no projeto. Além disso, decisões são tomadas com base em modelos econômicos que descrevem apenas um momento no tempo e não passam informações sobre possíveis cenários alternativos. Este trabalho objetiva desenvolver e demonstrar uma metodologia que pode auxiliar times de projeto na tomada de decisões e planejamento de recursos através da análise de risco econômica de projeto utilizando simulações de Monte Carlo. Três exemplos foram construídos para exemplificar o método; o primeiro é uma avaliação da integração de uma planta de biobutanol a uma usina de cana de açúcar existente, constituindo uma biorrefinaria, o segundo é a análise de um processo de produção de ácido mucônico a partir de biomassa usando pouca quantidade de informação, e o terceiro é a avaliação de uma tecnologia de produção de açúcar lignocelulósico e seu potencial como fornecedora de matéria prima para a química renovável.

Os resultados mostram que uma integração de biorrefinaria, um processo e mesmo uma proposta de tecnologia podem ser avaliados com sucesso através da análise de risco econômica, a probabilidade de se atingir um determinado resultado econômico pode ser calculada e os principais fatores que influenciam nos resultados podem ser claramente identificados. Conclui-se que a análise de risco através de simulações de Monte Carlo é uma ferramenta importante a ser usada em projetos de química renovável.

Palavras-chave: Biorrefinaria, Análise Técnico-Econômica, Análise de Risco, Monte Carlo

Abstract

At the early stages of projects of chemical process, decisions are taken based on the previous knowledge and past experiences of the people involved. Business decisions to go on, stop, or modify the project plan are based on economic models that describe a frozen photograph in time, and don´t provide sufficient insights on alternative scenarios. This work intends to develop and demonstrate a methodology that could help in the project decision making process and in the allocation of development resources. This methodology is based on the economic risk analysis of a project by using Monte Carlo simulations. Three examples were presented in this work in order to test and exemplify the method; the first makes an assessment of feasibility of the integration of a biobutanol plant as an added-on facility to an existing sugarcane mill constituting a biorefinery. The second, is the evaluation of the feasibility of manufacturing muconic acid from biomass using low level of information available, and, the third, is the analysis of a lignocellulosic sugar production technology and its prospect as raw material provider for renewable chemistry.

The results show that a whole biorefinery integration, a single process and even a single technology proposition can be successfully assessed through the economic risk analysis; i.e, the probabilities of achieving desired economic results can be calculated, along with the expression of the main factors influencing the results, allowing to conclude that the economic risk analysis using Monte Carlo simulations is an efficient tool to be used in renewable chemicals production projects.

Keywords: Biorefinery, Techno–Economic Analysis, Risk Analysis, Monte Carlo Simulation.

FIGURE INDEX:

TABLE INDEX:

LIST OF ABBREVIATIONS:

Opex: Operation Expenditures

Capex: Capital Expenditures

CHP: Combined Heat and Power

ABE: Acetone, Butanol and Ethanol

BuOH: Butanol

EtOH: Ethanol

MA: Muconic Acid

CW: Cooling Water

CWR: Cooling Water Return

R&D: Research and Development

NPV: Net Present Value

IRR: Internal Rate of Return

EBITDA: Earnings Before Interest, Tax, Depreciation and Amortization

FMC: Full Manufacturing Cost

ROCE: Return Over Capital Employed

ISBL: Inside Battery Limits

OSBL: Outside Battery Limits

PNA: Programa Nacional do Álcool (National Ethanol Program)

NREL: National Renewable Energy Laboratory

CEPEA: Centro em Estudos Avançados em Economia Aplicada (Center for Advanced Studies in Applied Economy)

BLS: Bureau of Labor Statistics

ANSI: American National Standards Institute

AACE: American Association of Cost Engineers

LIST OF UNITS:

kt/y: Kilotons per year

US$/t: Dollars per ton

MUS$: Millions of Dollars

kUS$: Thousands of Dollars

dt: Dry tons (of a solid)

Summary

1. CHAPTER 1 – INTRODUCTION

1.1. Problem Statement

The objective of this work is to help identify business plan actions for economically attractive integration of renewable chemistry processes into existing sugar and ethanol mills in Brazil. Through an early stage proposed project analysis, it helps to identify the key aspects that might leverage or kill the project, as well as determining the possibilities of achieving the desired economic results. In order to evaluate the biorefinery project and define the development actions, risk analysis techniques will be employed to evaluate the possibility of a given economic result being achieved by the project, and to identify the leverages that would increase the chances for a successful project or the pitfalls that would stop this same project.

To validate the proposed method of analysis, technical and economic feasibility of a bio n-butanol production project will be evaluated and stochastic risk analysis of such process will be performed. Mass and energy balances and specific consumptions will be calculated, operational and investment costs will be estimated, and then, variations of the main process and economic variables will be assigned in order to perform the risk analysis. The sugar and ethanol mill should supply the material and energy needs of the integration, and the impacts of the adding of a new process in the outputs of the mill will also be analyzed, for example, in the production of sugar and ethanol, the need to buy biomass from an external source and the related economic impacts. This work evaluates the attractiveness of building a biorefinery from an existing sugar and ethanol mill in Brazil and adding a technology for the manufacturing of n-butanol.

To further exemplify the range of the method, the process for production of muconic acid from biomass will also be considered, to show that it is possible to conduct an economic and risk analysis using any level of information that the investors may have. The primary source of information for this analysis is a patent filed by a technology company, and a fair portion of the process is designed with low level of detail, showing that in spite of the uncertainties in the process, the results of the risk analysis are sufficient to evaluate feasibility, the leverages and the killers of the project.

Also, in a third demonstration of the methodology, a biomass hydrolysis technology will be evaluated as a platform for the production of renewable chemicals through stochastic risk analysis. The methodology will be used to determine the potential price of the chemicals derived from the lignocellulosic sugars and their potential market fields.

The method proposed in this work helps to improve the decision making process even when the technical data is not available in detail. The economic and risk analysis can be as complete as desired to include competitiveness evaluations, market evaluations, etc.

This work is about facilitating project decision making through the use of a proposed methodology and the elaboration of an algorithm for economic and risk analysis is outside the scope.

1.2. Context

Many companies have recently considered biofuels and chemicals produced from renewable raw materials as products do diversify their portfolio, reduce the environmental impact and as a niche market that could pay a prime price for environmentally friendly and sustainable manufacture. Key markets include fuels, cosmetics, food and intermediate chemicals.

Sugar and ethanol mills are the best candidates to become the main base for the construction of biorefineries in Brazil. There are more than three hundred sugar and ethanol mills operative in the country; recently big food and energy players such as Shell, BP (British Petroleum), Bunge and Cargill have been investing in brazillian mills. Sugar cane is an established culture that already provides renewable raw material for the production of sugar, fuel and industry grade ethanol and energy, among its advantages is the fact that it also yields a fair amount of lignocellulosic raw material and does not compete with food crops as is the case with corn.

Furthermore, a wide array of technologies and processes to produce biofuels and renewable chemicals are being developed by start-up companies around the world (start-ups are young companies that develop technologies, usually in bench scale, and look for investors and partners in order to hasten scale up and development). Companies that do business in sugar and ethanol, energy, food and chemicals are potential partners to these start-ups since they detain the raw material supply chain, the market knowledge, influence and the investing power. Still, there are a number of companies outside these markets such as banks, automotive companies and others, which have the investing capacity also to partner with these start-ups.

For a sugar and ethanol mill, there is value to be added through integration of its processes into a biorefinery. During the first decade of this century in Brazil, the great demand for fuel ethanol due to the mass production of “flex fuel” cars led to an increase in investments in ethanol plants, but the first generation ethanol production from sugar cane juice faced competitiveness issues due to the gasoline price regulation in the country, causing the sugar and ethanol companies to acquire big debts (Brasil Econômico, 2014). In this sense, the diversification of products became an alternative for these companies in this scenario.

Many partnerships between start-up biotech companies and sugar and ethanol companies have been established in Brazil, such as the partnership between Amyris and sugar and ethanol group São Martinho, Iogen with Raízen for biomass hydrolysis, Solazymes with Bunge to develop the production of oil from algae fermentation, and the partnership between Cobalt and the chemical company Solvay to develop the production of n-butanol from lignocellulosic sugars. What makes a partnership with a start-up appealing for big companies is the possibility to access the new technologies as well as lab and specialized researchers at a more mature state then it would be possible if they have started the research by themselves.

Although partnerships with start-ups offer attractive opportunities, it also presents considerable risks. Most sugar and ethanol companies’ don´t have a specific budget for research and development, and even in the case of big companies that do have it, errors in management might lead to catastrophic consequences. Biotech projects often involve huge investments for piloting and demo plants, because they involve new applications of technologies, and due to the dilute aspect of many processes, low yield from biomass to products and low biomass densities that result in large scale equipment design even in pilot plants.

Start-up companies present their projects to prospect investors and partners usually at a concept stage; maturity of the technology is usually at a bench scale of development. In biotechnology, scaling up is a big challenge, especially for applications such as biofuels, where the scales of production needed results in processes of very large proportions.

For biorefineries, three large classes of risks can be defined; the first is the market risk, a lot of the proposed products to come out of biorefineries do not have a defined market or a clear definition for its price, in the case of biofuels, the revenues may not be enough to provide a scale large enough to make the project feasible. The second class of risks is related to the use of biomass as feedstock. Although every source of biomass has the same building blocks (cellulose, hemicellulose and lignin), each biomass has different processing characteristics, for instance some have a high variation in moisture and impurities and biomass availability depends on climate in some cases. A third class of risks relates to uncertainties within the process development itself, where many of the technologies proposed for the production of the renewable chemicals are mature for just a few products, and a lot of the developments are still in bench scale (Hÿtonen, et al., 2012).

1.3. Objectives / Work Proposal

In the early stages project development, the identification and management of the project´s risks is important to avoid pitfalls and wrong investments at bench scale, piloting and demo of a process in development. Investing a big sum of money in human resources and equipment for a pilot or demo plant only to deem the process unfeasible afterwards can have catastrophic consequences for the companies involved; going from financial problems to the bankruptcy of the ventures leading to a lack of motivation to keep research in renewable chemistry and biorefineries.

The scope of this work is to present tools, and a methodology to organize actions in such a way to aid project teams to make the right decisions early at conceptual stages of projects to integrate new processes into biorefineries, by estimating the probability of the project to achieve a desired economic result and by identifying the main drivers or killers of the project that should be addressed to increase confidence on the results, one could make decisions on whether to continue or interrupt a project development, aid the project development experimental planning, reduce risk levels in each new project stage and, finally, increase the confidence in the economic figures of the project as the development unfolds.

The advantage of building a model for the process and identifying the risks right at early stages is to be able to develop a research plan that may reduce uncertainties as the project unfolds. In most partnerships between startups and chemical or sugar and ethanol companies, the process proposed is generally in its early stages of development, at the bench phase or, sometimes, at pilot scale. In this scenario, the startup intends to reduce the risks of scaling up by sharing with a partner the investments in pilot and demo scales, avoiding big debts that could trouble the company. On the other hand, big companies look to partnerships in search of new technologies with the objective of gaining an advantage over the competition by securing new markets, especially those willing to pay premium for renewable or green chemicals, or by filing patents, assuring exclusive exploitation of the technology.

As a base for the process add-on into an existing mill site, a regular Brazilian sugar and ethanol mill will be used as model. Microsoft Excel software will be used to build the mass and energy balances for both the mill and the proposed processes and Economic and Risk analysis will be performed also in Excel with the use of the software @Risk from Palisade.

A biobutanol production process through ABE (Acetone, Butanol and Ethanol) fermentation will be used as model for the economic and risk analysis. A mass and energy balance will be built for the process starting from a lignocellulosic raw material pretreatment to media preparation, fermentation and downstream separation. Also, a mass and energy balance for the sugar and ethanol mill receiving the biobutanol plant as annex will be developed, along with a combined heat and power system that will be producing steam and electricity to attend both the mill´s and the biobutanol plant´s demands. Excess electricity production will be sold to the grid as it happens in current facilities producing sugar and ethanol.

In order to further demonstrate the method, a muconic acid production process was analyzed; the objective is to show the feasibility of using a risk analysis to analyze a process that is less comprehended than the biobutanol production.

The risk analysis was also tested in the evaluation of a processing technology instead of a full process or a project: the evaluation of a biomass hydrolysis technology.

1.4. Work Organization

In Chapter 1, the contextualization of the work and the objectives are presented.

In Chapter 2, the sugar and ethanol mill is discussed regarding the configurations, history and the process, along with concepts on biorefineries, the categories and feasibility. A literature review on the state of the art of biorefinery analysis is also presented, and fundamentals on economic and risk analysis are also discussed.

In Chapter 3, the tools and methods used for building the models, the technical economic analysis and the risk analysis tools are described.

In Chapter 4, the tools and methods presented will be used in the analysis of a biorefinery project using a sugar and ethanol mill as base in Brazil. The technical economic analysis of the biobutanol plant and the transformation of a sugarcane mill into a biorefinery with the biobutanol plant will also be analyzed. A risk analysis will be performed with the objective of unveiling the probabilities of attractive economics and finding out the leverages and barriers that should be prioritized in the project development.

In Chapter 5, a second case is studied to reinforce the applicability range of the methodology: a process to produce muconic acid from biomass is evaluated using a patent as information source, this example serves two purposes: to show that the method is feasible in very early stages of a project, with very little information available and to demonstrate the value of the risk analysis in this scenario.

In Chapter 6, the technology for the transformation of biomass into lignocellulosic sugars is evaluated by its potential to yield sugars as intermediates for the production of biofuels and chemicals.

In Chapter 7, conclusions about the methodology and its performance in terms of providing useful information to the project decisions will be analyzed.

A schematic organization of this work is shown in Figure 1.1.

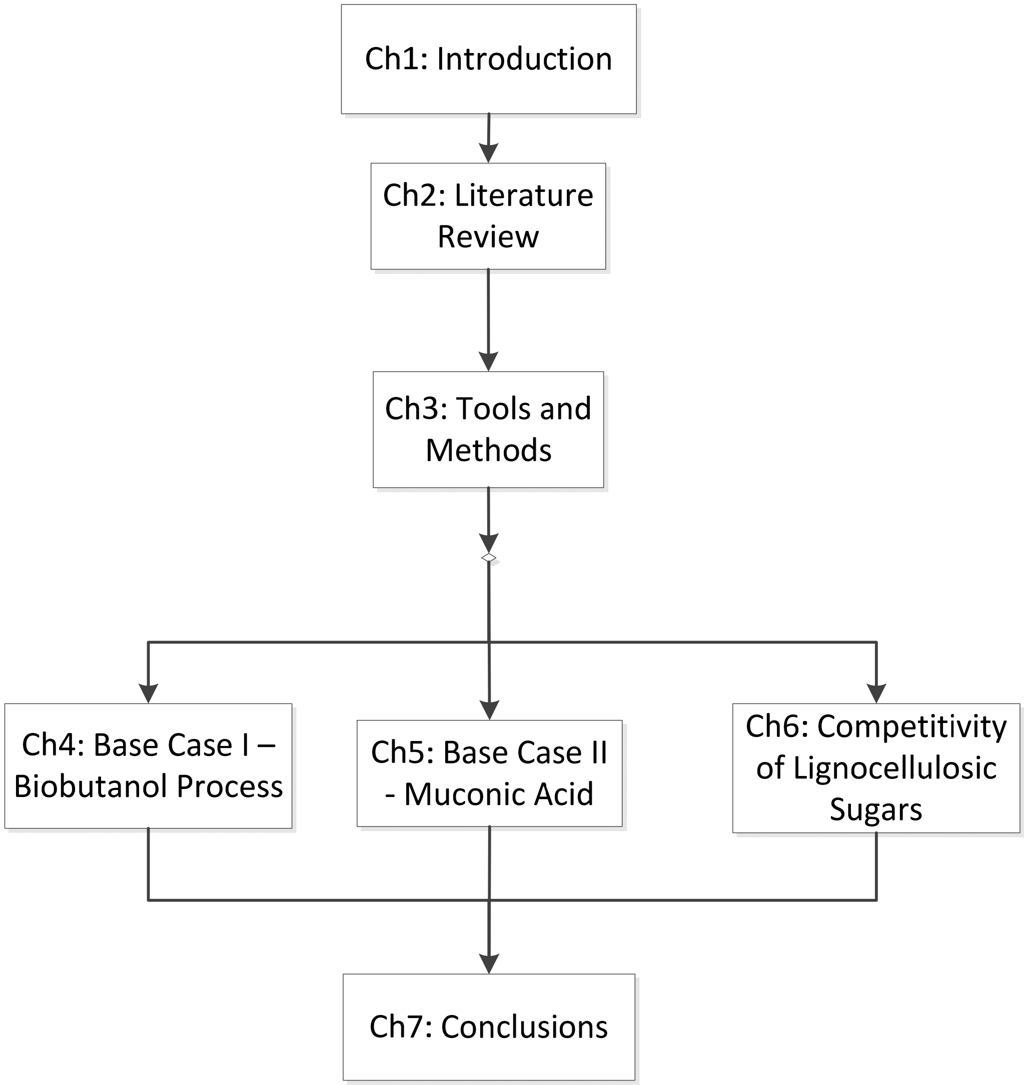


Figure 1.1 General Structure of the Dissertation

2. CHAPTER 2: LITERATURE REVIEW

2.1. Sugar and Ethanol Mills: General Configurations

The sugar and ethanol production is well spread throughout Brazil, there are over three hundred sugarcane processing facilities distributed mainly across the southeast, middle east and northeast regions. There are three main types of mills:

- ethanol mills (autonomous distilleries);
- sugar mills and;
- sugar and ethanol mills.

The latter type is the most common and accounts for most of the production in the country.

Table 2.1 shows the mills distribution in Brazil by region.

Table 2.1 Distribution of the Different Types of Sugarcane Mills in Brazil - Translated from Conab (2008)

Region	Sugar and Ethanol Production Units	Ethanol Production Units	Sugar Production Units	Total Production Units
Number of Production Units				
Center-South	176	81	7	264
North-Northeast	49	23	7	79
Brasil	225	104	14	343
Grinded Sugarcane in the 2007/08 Season (in kton)				
Center-South	367,539	51,680	6,468	425,687
North-Northeast	49,569	8,173	4,735	62,476
Brasil	417,107	59,853	11,202	488,163

In the next paragraphs these configurations are discussed with further details.

2.1.1. Ethanol Mills (Autonomous Distilleries)

In autonomous distilleries, sugar cane is processed in a series of mill tandems or in a diffuser for sugar cane juice extraction, the juice is treated with the use of decanters and filters for removal of impurities such as waxes (contained in the sugar cane) and dirt (dragged by the crop system). The filter cake from filter process is recycled to the sugarcane fields. Treated sugar cane juice is concentrated in evaporators to adjust the sugar concentration to the fermentation process.

In the fermentative process, yeast *Saccharomyces cerevisiae* is used to transform sugar into ethanol in fed batch or continuous mode. After fermentation, the yeast is separated from the beer by centrifuges, and then sent to a treatment designed to reduce contamination and maintain cell viability so it can be recycled back to the production fermenters. The centrifuged beer is then sent to the distillation set.

Distillation for hydrous ethanol production is carried out mainly in two distillation columns in a stacked configuration, the first serving as ethanol stripping from the beer and the second as a rectifying column to produce ethanol in its azeotrope composition. Some mills produce anhydrous ethanol through azeotrope distillation with cyclohexane, extractive distillation with monoethylene glycol and molecular sieves. The ethanol distillation process also generates vinasses, composed of water, residual sugars, cells from the fermentation process, salts and other organic matter. Further information on ethanol producing mills can be found elsewhere (Ensinas, 2008).

2.1.2. Sugar Mills

In the sugar manufacturing sugarcane mills, the juice is extracted with mill tandems and treated in a similar way to the distilleries, but with some important differences. In an attempt to reduce color formation in the sugar, the sugarcane juice is treated with sulfur dioxide generated by the burning of elemental sulfur. The stricter is the color specification for the sugar, the more sulfur is necessary in the juice treatment.

The treated juice is then sent to evaporators to concentrate the juice almost up to the saturation point of sugar, the concentrated sugar juice is called syrup. Juice concentration is generally carried out in multiple effect evaporators that also provide energy to other parts of the process through bleedings in the vapor lines out of the first and second effects. In a multiple effect evaporator system, a pressure gradient is forced through five or six stages of concentration, meaning that the water boiling temperature is always lower in the subsequent effects, so vapor generated in one effect carries enough energy and pressure to be used as drive for the next effect. With such configurations, it is possible to evaporate up to five or six tons of water for each ton of steam consumed, depending on the number of effects used.

The syrup is then sent to the crystallization section, where it is concentrated above its saturation point and seeded to promote formation of sucrose crystals. The crystallized mass is centrifuged, separating the crystals from the molasses. The crystallization process is carried out in a countercurrent stage scheme driven by the mass purity (sucrose percentage of total dissolved solids). After crystallization, sugar crystals are centrifuged, dried and either sent to a silo or to a packaging plant. Molasses generated in the final stage still contains considerable amount of sucrose, but the low purity makes it uneconomical to further and crystallize it, in sugar only plants, molasses is sold for fermentation in the food industries. Information about sugar producing mills can be found elsewhere (Rein, 2007).

2.1.3. Sugar and Ethanol producing mills

In most sugarcane mills in Brazil, both sugar and ethanol processes coexist in the same plant. There are interesting synergies to be considered including the use of the molasses for ethanol production, the use of vapor from the concentration system to drive distillation and the possibility to control the diverted sugar to fermentation in order to optimize the mill´s economics. Figure 2.1 shows a diagram for a typical sugar and ethanol producing sugarcane mill.

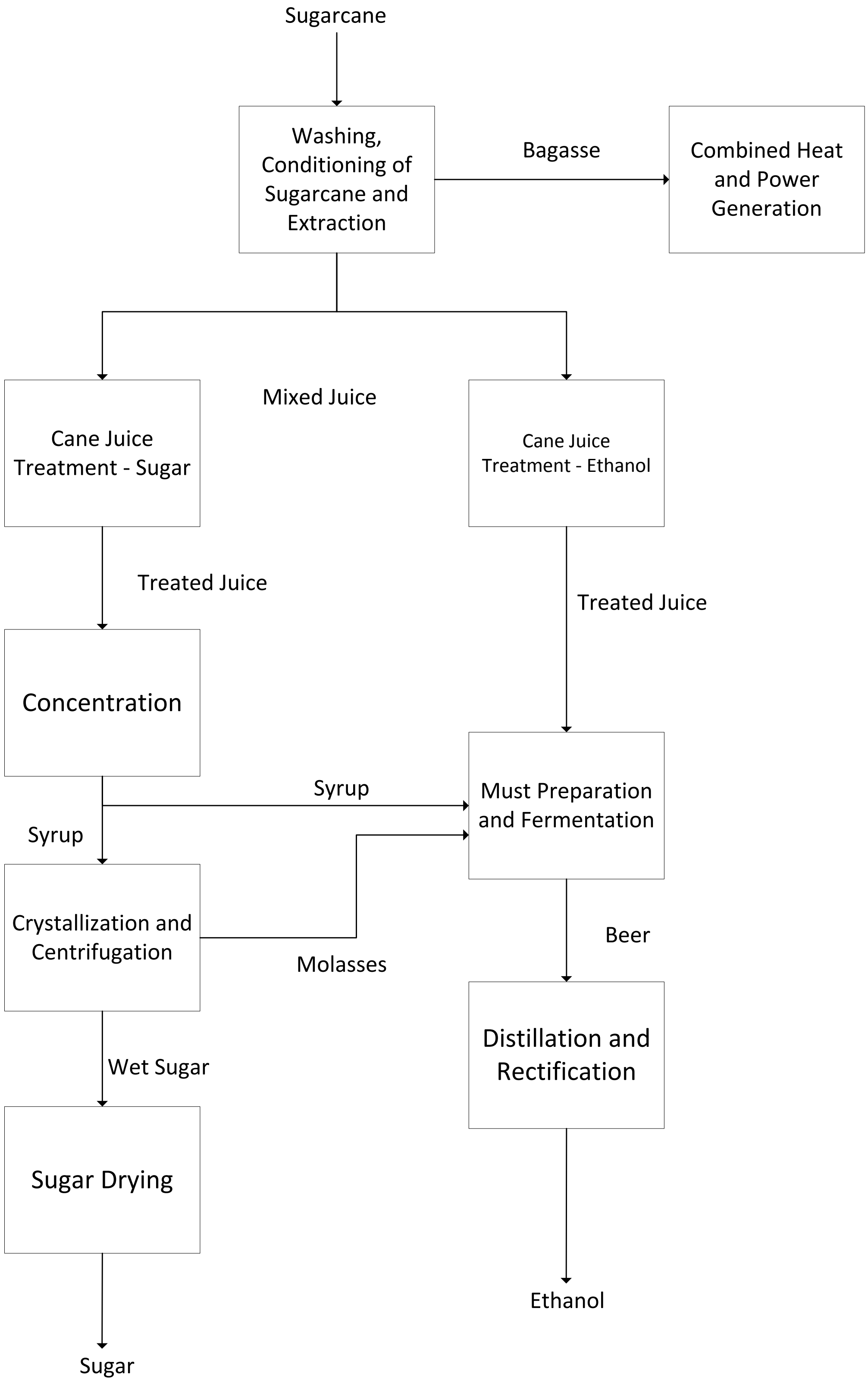


Figure 2.1 Block Diagram of a Sugar and Ethanol Mill - Adapted from Ensinas (2008)

2.1.4. Sugar and Ethanol Mill Process Steps

In this section, the process of a sugar and ethanol mill that serves as basis for the biorefinery studied in this work will be described. Each process step will be presented with the configuration premises considered. Figure 2.2 shows a typical sugarcane mill process diagram.

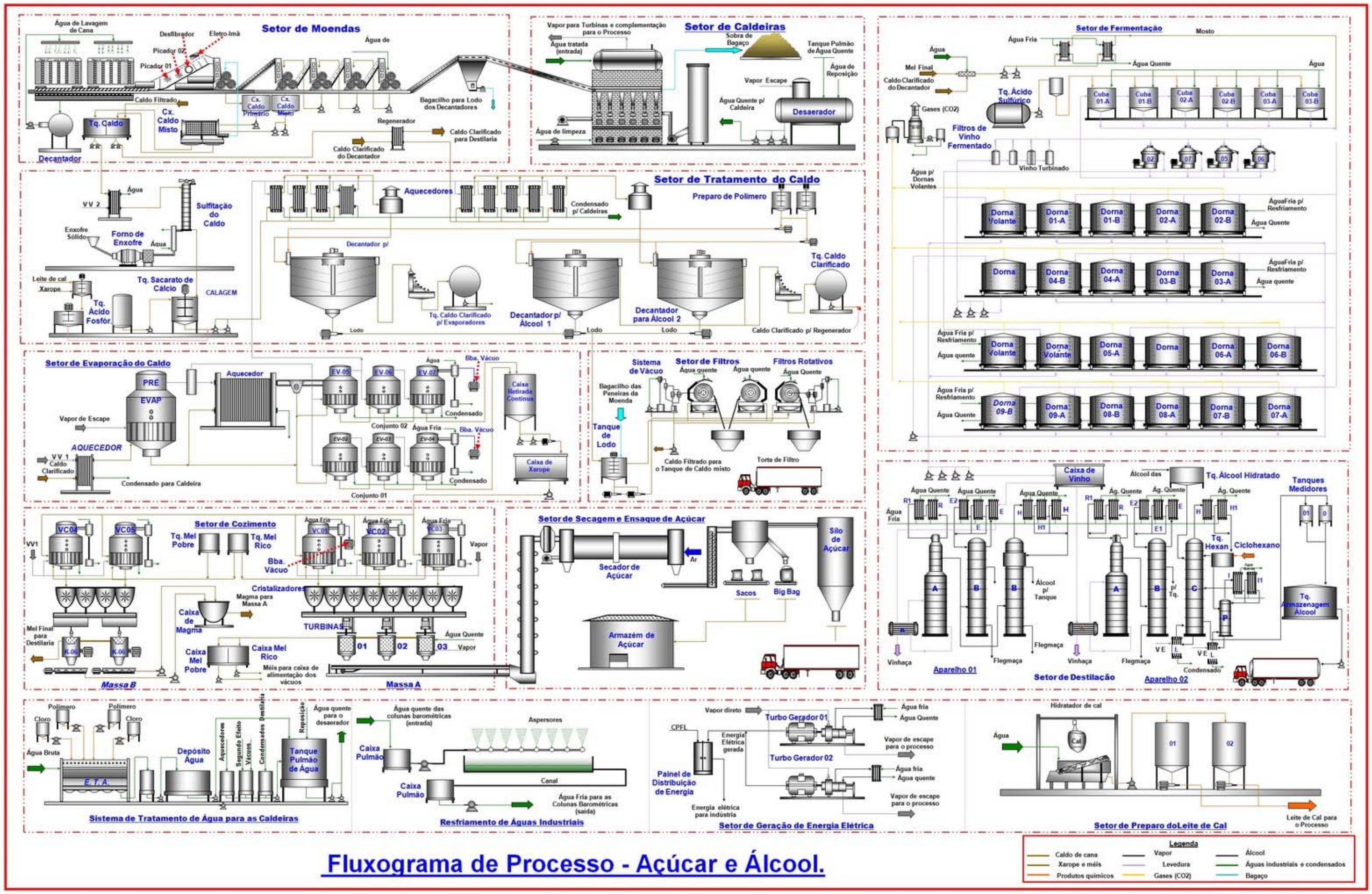


Figure 2.2 Typical Mill Diagram

2.1.4.1. Grinding

Grinding is the first processing step inside a sugar and ethanol mill, the sugar cane disposed by trucks in conveyors is cleaned either with air blown by fans or with water, though water washing is being discontinued due to the considerable sugar losses involved.

After washing, the sugarcane is chopped and shredded by a set of hammers in preparation for the actual grinding of the fibers. The cane fibers go through a set of four to six tandems in series where it is crushed to separate the juice with sucrose from the fibers.

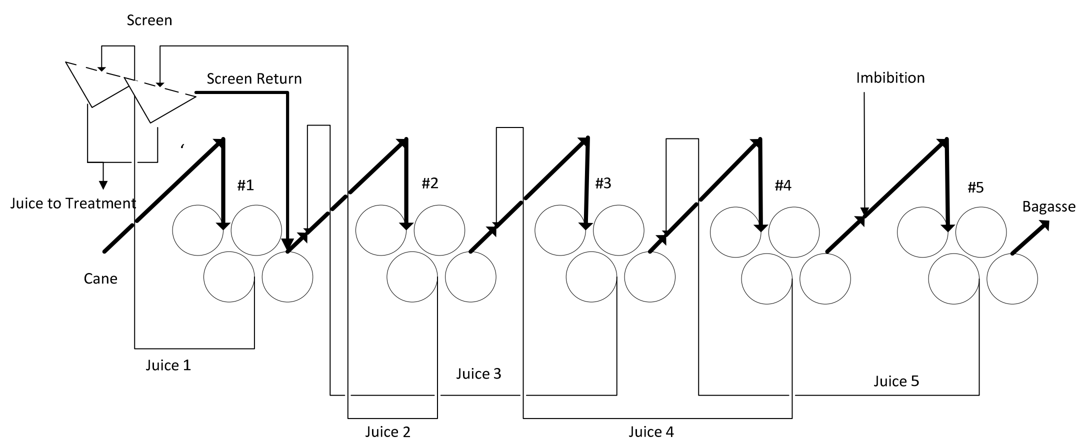


Figure 2.3 Sketch of a Grinding Process – Adapted from Rein (2007)

As shown in Figure 2.3, while being crushed in mill tandems disposed in series, the sugarcane is washed in counter current, fresh water is injected in the sugarcane right before the last tandem crushing, the juice from the last tandem is injected in the sugarcane before the crushing in the preceding tandem, until the second tandem juice is obtained. The juice from the second tandem is screened for coarse solids and sent to juice treatment, in the first tandem there is no washing required, the juice from the first tandem is also screened and sent to juice treatment.

Further information on sugar cane crushing process can be found elsewhere (Rein, 2007).

2.1.4.2. Juice Treatment

After grinding, the sugarcane juice containing sucrose is sent to the juice treatment plant, the objective of this part of the process is to remove dirt, wax, and other solids contained in the juice and prepare the juice for the sugar production. The sugarcane juice is treated with lime and sulfur dioxide, clarified and heated. The mud from the clarification process is filtered for sugar recovery and the filter cake is sent back to the field as fertilizer. Specifications of the process, e.g. the amount of lime and sulfur used is defined according to the type of sugar produced in the mill and if the juice will be used for production of ethanol instead of sugar. Figure 2.5 shows a sketch of a process to clarify the sugarcane juice.

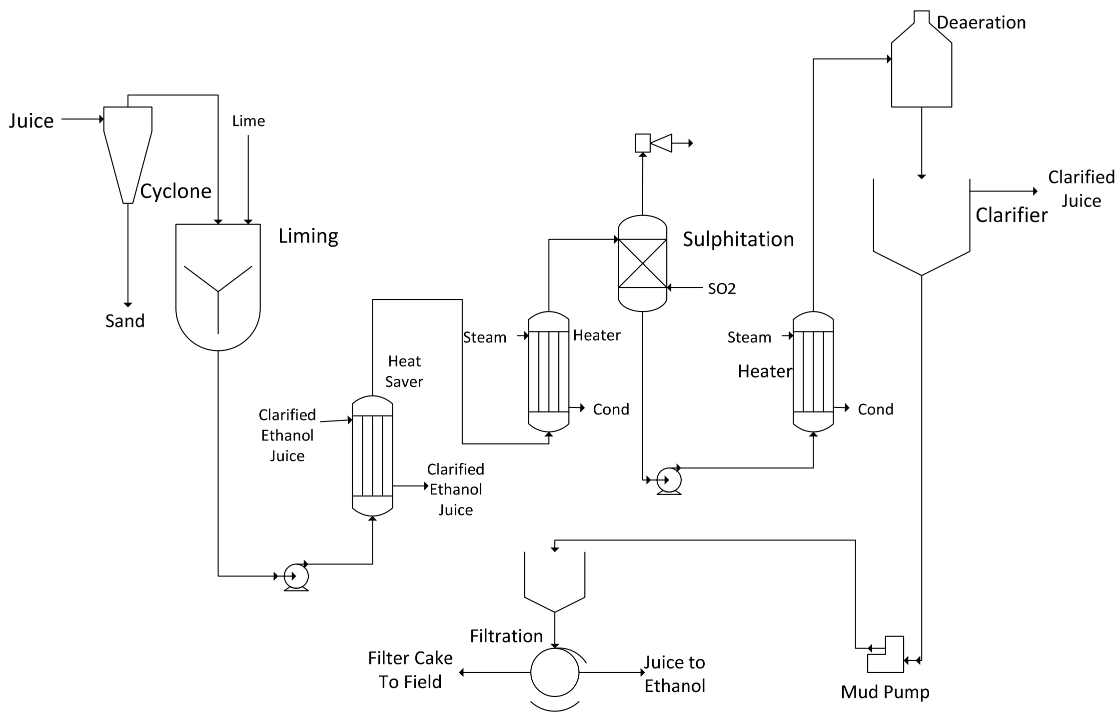


Figure 2.4 Sketch of a Juice Treatment System

Further information on the juice treatment process can be found elsewhere (Rein, 2007).

2.1.4.3. Sugar House

Sugar production starts with the concentration of the clarified sugarcane juice, the objective is to bring juice concentration up to the saturation concentration (approximately 65% in mass). The juice concentration is carried out in a multiple effect evaporator, a concentration method where a pressure gradient is applied to evaporators disposed in series and the vapors from one evaporator is used as driving force for the next one. Figure 2.5 shows a sketch of a multiple effect concentration system.

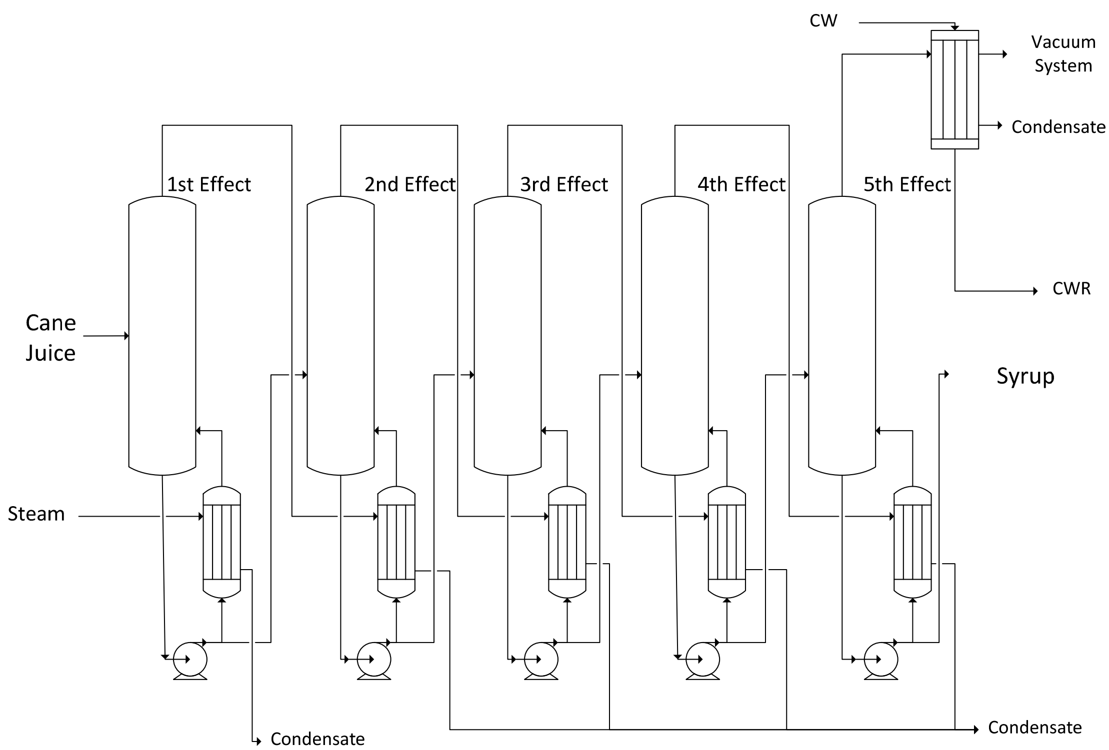


Figure 2.5 Sketch of a Juice Concentration System

After concentration, the syrup formed is sent to the crystallization process, which is carried out in crystallizers or pans, and then centrifuges separate the sugar crystals from the molasses. Crystallization process occurs in stages, the crystals formed in the C Pans (Figure 2.6) are separated in the centrifuges yielding molasses and C Sugar, that is sent to the A Pans where crystallization is continued until the final sugar crystals are reached. The crystallization media is then separated again by centrifugation and the sugar is dried and sent to storage, the molasses separated in this centrifugation, still containing an important amount of sugar is sent to the C Pans. Figure 2.6 shows a sketch of a sugar crystallization system.

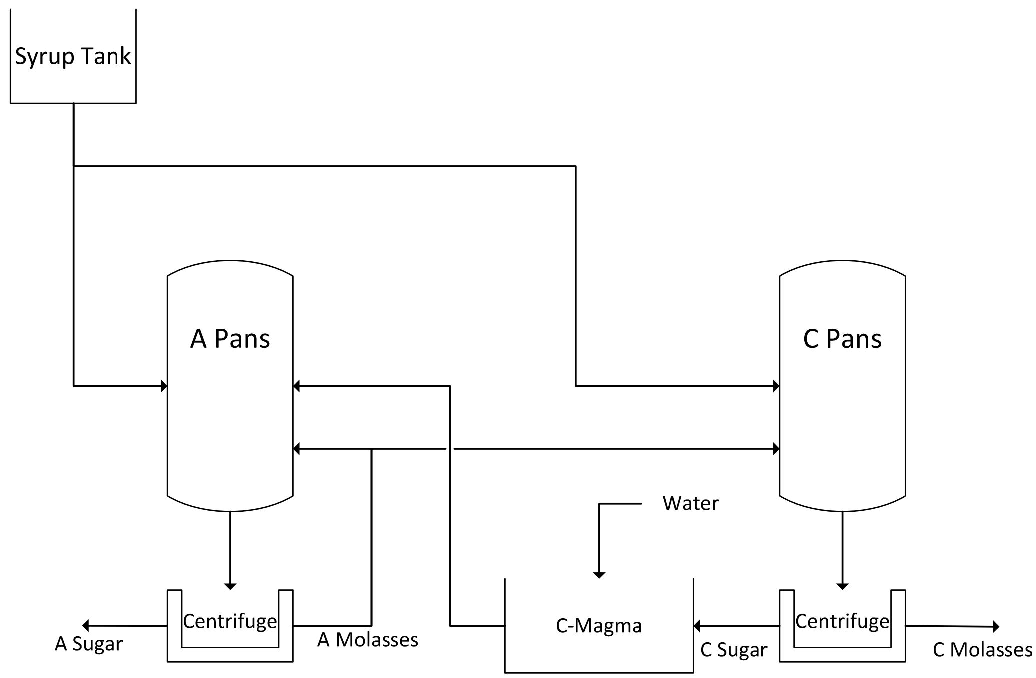


Figure 2.6 Sketch of a Sugar Crystallization System – Adapted from Rein (2007).

Further information on the crystallization process can be found elsewhere (Rein, 2007).

2.1.4.4. Fermentation

In the sugar cane mills that produce both sugar and ethanol, the molasses produced in the sugar factory and part of the clarified juice is sent to the fermentation process. In the fermentation process, sucrose is converted into ethanol by the *Saccharomyces cereviseae* yeast. The process consists of production fermenters and a yeast treatment process, where yeast is separated and recycled in the process. Fermentation gases are sent to a scrubber where ethanol is recovered with water. Figure 2.7 shows a sketch of a fermentation process.

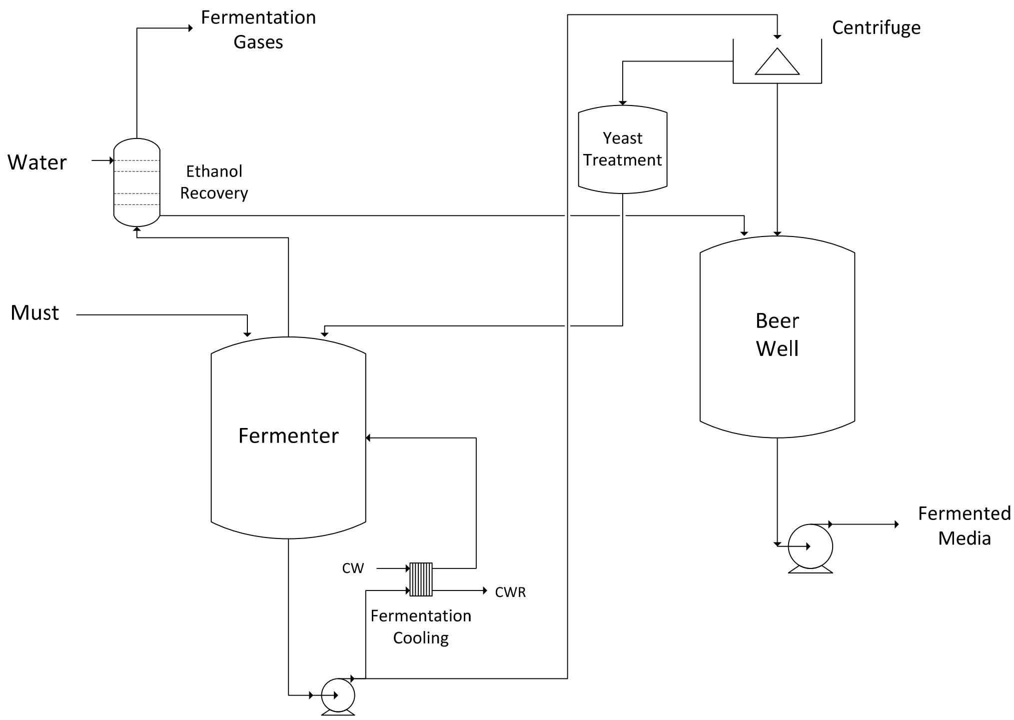


Figure 2.7 Sketch of an Ethanol Fermentation System

2.1.4.5. Distillation

After fermentation, the fermented media, or beer, is sent to separation in distillation columns, two columns in series are used to produce the hydrous ethanol, which is ethanol at its azeotrope, which happens at an ethanol concentration of around 95%. In the first column, the beer stripper, ethanol is separated from the beer yielding the phlegma, an ethanol spirit with a concentration of around 40% and vinasses, which is composed of water, salts, heavy organic compounds produced in fermentation and other solids. In the second column, called rectification column, which usually operates in a stacked configuration with the beer stripper (Figure 2.8), the hydrous ethanol is obtained.

Figure 2.8 shows a sketch of a distillation system.

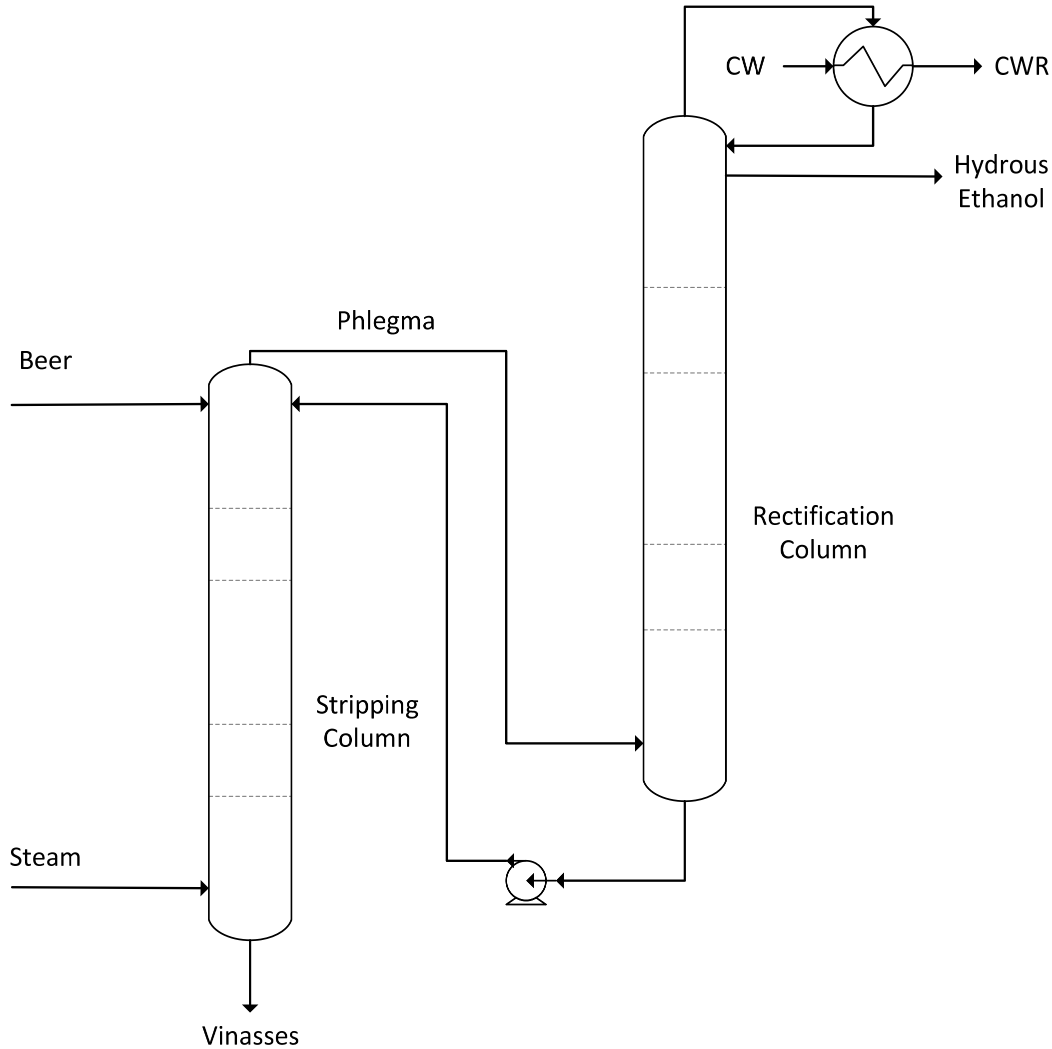


Figure 2.8 Sketch of a Distillation System – Adapted from Batista (2008)

Further information on distillation can be found elsewhere (Batista, 2008).

2.1.4.6. Combined Heat and Power

Sugar cane mills are usually self-sufficient when it comes to heat and electricity during the grinding season. The bagasse left from the milling process is used as fuel and has heating energy sufficient to drive all the mill´s processes and in most cases, excess energy is generated for export.

Bagasse is transported through conveyors from the milling tandem to the boilers where it is burnt to generate steam in pressures varying from 65 to 100 bar, steam is primarily used as driving media for condensation and counter pressure steam turbines, the electricity generated is used in the production process and excess is sold to the grid.

Exhaust steam from counter pressure turbines, at pressure around 2.5bar.a is used in the sugar production process in the heating and concentration of green juice after treatment. Concentration of juice is done in a multiple effect system, in which a pressure gradient is forced across a number of evaporators in series in order to make it possible that the vapors from one evaporator serve as driving force for the next. This configuration of evaporators also serve as a vapor distribution center for other processes of the mill such as sugar crystallization and ethanol distillation, providing an increased energy efficiency of the mill.

In older mills there are still boilers generating steam at 21bar.a, this steam is used for shaft work in the cane mill tandems, in the diffuser, cooling water and cane washing water pumps, systems that move big volumes of water. In the mills built after 2000, the single stage turbines that provided shaft work were substituted by more efficient electrical motors.

A bagasse reserve of 7 to 10% of the total is usually separated to provide energy during the startup of the mill in the beginning of the season and when the production has to be stopped due to shortage of sugar cane or impossibility of harvesting due to rain.

In the last twenty years, the mills have generated electricity not only for internal use, but to selling to the grid as well, creating momentum for investment in modernization projects, energy efficiency and expansion projects. Another important change due to the surge of this new market has been the creation of strategies so the combined heat and power (CHP) section of the mill operates longer than the crop season time mainly through bagasse and straw storage.

The need to generate electricity year round together with the prohibition of burning the sugar cane fields prior to harvesting led to another important change in the sugar cane industry: The recovery of the sugar cane straw from the field to be brought to the mill and its use as fuel together with bagasse. Using the cane straw as fuel has advantages and disadvantages over the use of bagasse, the disadvantage being the presence of impurities and the advantage its lower water content.

Sugar cane straw is collected in the field after harvest in bundles made by specially designed machines, at the mill, the bundles are undone, the straw is clean and chopped, the making of bundles is an important step of the process that affects directly logistics costs and thus affects the cost of the raw material to the process.

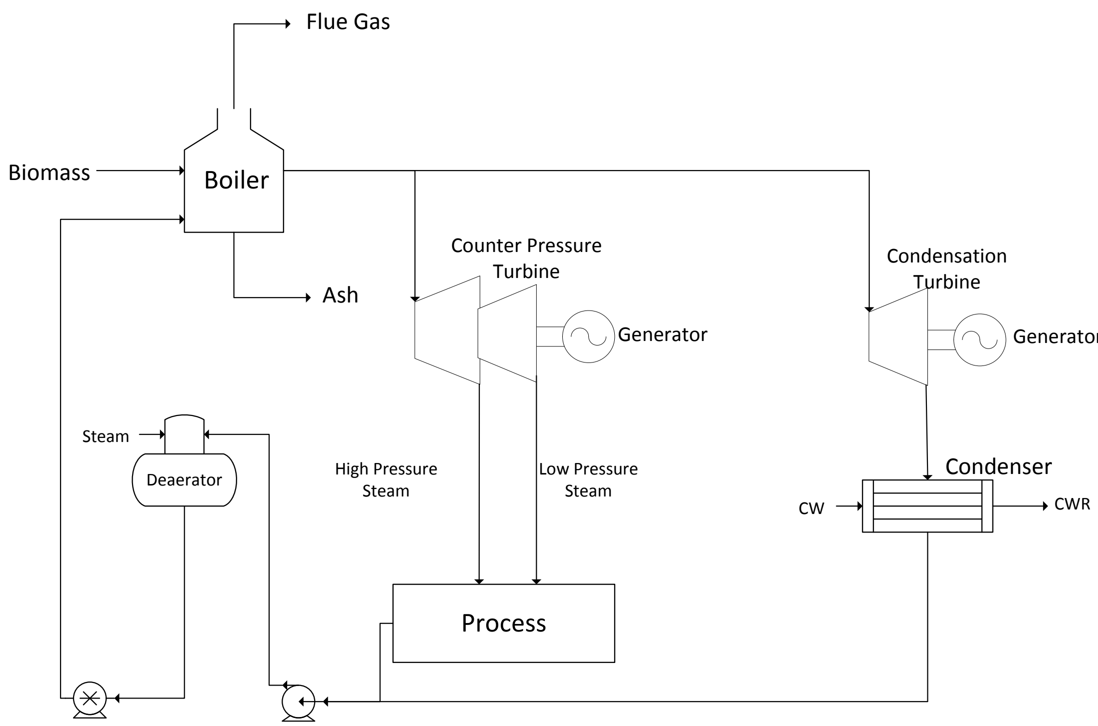


Figure 2.9 Typical Configuration of a Mill´s Combined Heat and Power System

2.2. Sugar, Ethanol and Biorefineries – State of the Art and Perspectives

2.2.1. Recent history of sugar and ethanol production

Until the decade of 1970, sugar cane was mostly used for sugar production, after the first oil crisis in 1973, the Brazilian government created the PNA, *Programa Nacional do Álcool* or national ethanol program, and in 1975 the "Proalcool", aiming at fomenting the production of anhydrous ethanol to be used as an additive to gasoline from the residue of sugar factories. The Proalcool program was based on three main policies: parity of sugar and ethanol prices, guaranteed purchase of all ethanol produced by the state owned oil company Petrobras, and an industrial and agricultural credit line for the program (Lanzotti, 2000).

In the first phase of the Proalcool program, the feedstock for ethanol production was mainly molasses generated as residue in the sugar factories that was fermented and distilled to produce anhydrous ethanol serving as antiknock additive in gasoline. In the second oil crisis in 1979, as the oil barrel price spiked from US$ 12.5 to US$ 30, the Brazilian government launched the second phase of Proalcool, promoting the production of hydrous ethanol at the mills and its use as an independent fuel in light cars (Carvalho, 2007). It was in this stage that autonomous distilleries emerged, using the raw juice from sugar cane as the feedstock for ethanol fermentation.

In the first half of the decade of the 80’s, the Proalcool program and ethanol production saw their best performance as the production of ethanol fueled automobiles increased steeply. In the second half of the decade, however, due to the deterioration of the country´s economy, ever increasing inflation, increase in debt, and with the reduction of the oil barrel price internationally as well as reduction in government subsidies, all these factors caused a decrease in investment in the Proalcool program and finally a shortage of ethanol in the market (Carvalho, 2007).

During the decade of 1990, production of ethanol remained stagnant and in the end of the decade the industry saw the reduction of its regulations, forcing producers to search for competitiveness leverages. In the decade of 2000, production of flexfuel cars brought the ethanol market back to life, causing a new rush of investments in ethanol producing sugar cane mills from private companies.

In the second half of the decade of 2000 and first half of the decade of 2010, ethanol growth stagnated, the number of projects for ethanol plants greatly reduced. Many reasons are pointed for such change in trend, amidst them are the increased production costs (land rent, consumables, crop mechanization and labor cost) and freezing of the gasoline price at the pump (Rodrigues, 2012).

2.2.2. Renewable fuels and products

During the first decade of the XXI century, environmental concerns together with oscillating oil prices and political instability in the regions of high production, led to the flourishing of projects and investments in technologies for production of fuel and chemicals from renewable sources to substitute the ones derived from oil.

In Brazil, the main renewable raw material sources are biomasses such as bagasse, sugar cane straw and oil sources such as those used for production of biodiesel. Research centers such as CTC (Centro de Tecnologia Canavieira), CTBE (Centro Tecnológico do Bio Etanol), IPT (Instituto de Pesquisa Tecnológica) as well as universities, among other institutions, have developed a relevant quantity of research in transformation of lignocellulosic materials such as bagasse and sugar cane straw.

In the decade of 2000, there has been big investment on biodiesel technology from several oil raw materials such as soy and mamona and also from grease residue from meat processing plants, these investments were done in the prospect of an increase in the allowed mix of biodiesel into regular diesel in Brazil. The investments in biodiesel were reduced as the perspectives of increase in the mixture were not materialized.

In the US, investments in biofuel research are connected to strategies of securing energy independence of imported oil. Research is usually done by both research centers such as de NREL (National Renewable Energy Laboratory) and by private companies, being most of them startups: newly born companies that develop technologies in small scales and then look for partners that can fund scale-up. Such partners range from medium and large industries to venture capitalists.

There is a huge diversity of biofuels and chemicals being researched to be produced from renewable sources, from oil and fuels such as ethanol to chemicals, specialties and materials. In one of its reports, NREL listed and ranked the molecules with the highest probability of achieving market success (NREL, 2004).

2.2.3. Biorefineries

There are a number of different biomass processing schemes that can be defined as biorefineries, Ree (2007) sorted and categorized different possible biorefinery configurations according to its raw materials and processes.

- Conventional Biorefinery, CBR
  - Separates biomass in its fractions, the biorefinery products;
  - Low variety of products;
  - The most common type of the plants currently in operation;
- Green Biorefinery, GBR
  - Based on compression of green biomass, yielding fibers and juice;
  - Fresh biomass is processed;
  - Depends on coordinated logistics with the crop fields;
- Whole Crop Biorefineries, WCBR
  - Work with cereal crops;
  - Based on dry or wet milling of grains;
  - Fibrous products as byproducts such as corn stover;
- Ligno Cellulosic Feedstock Biorefinery, LCFBR
  - Based on the fractioning of lignocellulosic raw materials;
  - High availability of low cost raw material expected in the future;
  - Might compete with food production;
- Two Platform Concept Biorefinery, TPCBR
  - Fractioning of biomass into sugars and lignin;
  - Sugar fraction converted to products by biotechnology processes, such as fermentation;
  - Lignin fraction converted by thermochemical processes;
- Thermo Chemical Biorefinery, TCBR
  - Thermochemical processes are used to convert biomass, such as torrefaction, pyrolysis and gasification;
  - A great range of products can be generated;
  - Process can be integrated into the Catalytic Stage Biorefineries;
- Marine Biorefinery, MBR
  - Use of algae and microalgae;
  - Good potential on carbon dioxide absorption;
  - In most cases needs lyse of the microorganisms.

2.2.4. Sugarcane mills as the base for biorefineries

The sugar cane used in the mills and the process of compressing and processing the juice puts sugar cane mills in the Green Biorefinery category according to Ree (2007), so sugar cane mills are already biorefineries even before integration with lignocellulosic biomass treatment processes. In the sugar cane mills, sugar cane is pressed, the juice is processed to produce crystal sugar and ethanol and the fibers are used as fuel for thermal energy and electricity generation. Sugar cane mills have potential for integration with other biorefinery processes due to the low cost sugar offer and the amount of lignocellulosic material available that can be cracked or thermally converted to pyrolysis oil or synthesis gas (Oliveira, 2010).

Oliveira analyzed the feasibility of projects for the installation of biorefineries based on sugar cane mills by first verifying which products are imported by the Brazilian market, being of interest for biorefineries and then evaluated its feasibility according to five requisites:

- Scale economy;
- Scope economy;
- Diversification;
- Diferentiation;
- Flexibility;

The installment of a biorefinery is more competitive than a standalone plant from the economy of scale point of view by the utilization of part of the available sugars for the production of different chemicals while sharing the infrastructure and utilities with the crystal sugar and ethanol processes. An important factor for the feasibility of such integration is adapting the utilities system for a year round production campaign versus the regular production season for sugarcane mills that is usually only two hundred days long per year.

Economy of scope is also existent in the production process of chemicals from sugars since the extraction stages of the sugars from the raw material are shared between the products, as well as utilities. In plants producing chemicals from ethanol, such economy is not always evident since there is the possibility of the chemicals plant consuming more ethanol than the fermentation of juice can produce, introducing the need to transport ethanol from another mill.

When a sugar cane mill puts forth an integration project to produce chemicals other than ethanol and sugar, it is diversifying its businesses by entering markets not explored before, it is also possible to diversify the raw materials by investing on the processing of corn stover for example. Contrary to diversification, what many companies search is verticalization of its businesses by dominating a higher share of its production chain, investing either in upstream or downstream operations.

Differentiation occurs when a company finds new niches of market for its products without changing the market itself. In the case of annexed biorefineries to sugar cane mills, differentiation may occur if second generation ethanol proves to be capable of generating a new niche of market due to its more favorable life cycle analysis (Oliveira, 2010).

In his work, Oliveira also determined key aspects to the feasibility of a sugarcane mill as base for a biorefinery, highlighted the main aspects of equipment occupation that can be increased by the higher quantity of operation days in the year, and the utilization of lignocellulosic material. The Table 2.2 shows the factors that leverage feasibility of a sugarcane mill as base for a biorefinery.

Table 2.2 Aspects that Leverage Sugarcane Mills as Base for Biorefineries – Translated from Oliveira (2010).

	Strategy	Sugar Chemistry	Ethanol Chemistry	Observation
1	Longer Campaigns	X	X	As the time of crop season increases, mean sugar content in the cane drops. There are also limitations of harvesting in rainy days.
2	Sugar Storage	X		Molasses or inverted sugar syrup could also be stored.
3	Ethanol Storage	X		Evaporation losses are a problem.
4	Integration with sugar and starch cultures	X	X	Industry investments needed. Technological challenges in agriculture. Raise in raw material costs.
5	Lignocellulosic Material Hydrolysis	X	X	Technology developments needed and availability of lignocellulosic raw material.
6	Thermochemical Routes		X	Technology developments needed and availability of lignocellulosic raw material.

A longer campaign, allowing the production throughout the whole year, reduces capital investment in new equipment and investment in product storage; on the other hand, it could mean higher investment in raw material storage of operation off crop season, such as molasses or sugars.

Integration to other crop cultures, being it sugar crops such as sweet sorghum or starch crops such as corn represents a diversification opportunity in raw materials as well as operation strengthening, since strong performance on one crop can compensate shortcomings on another. At the same time, diversification of raw material brings new challenges to the project, since crop seasons must be synchronized, meaning investments in land and in agriculture technology. This way, selection of crops to integrate with sugarcane must be done diligently according to strategies and plans of the biorefinery.

Sugarcane mills have great potential as base for a biorefinery integration since they generally have availability of lignocellulosic raw material to be processed both in thermochemical processes as well as in bioprocesses such as fermentation. Sugar can be used as raw material for the production of chemicals with high added value with fermentation and ethanol itself can be transformed into other chemicals. The mill also produces residues that can be used to generate value though digestion or algae production, excess yeast in ethanol fermentation can be used as nutrient for bacterial fermentations or can be processed and valorized as animal nutrition products, filter cake from juice clarification contain waxes produced by the sugarcane that can be extracted and valorized. From the energy point of view, the sugarcane provides the fuel to maintain the biorefinery operation in a self-sufficient mode.

It is important to study both the implementation of biorefineries using sugarcane mills in greenfield projects as well as the integration of biorefinery into existing sugarcane mills in the bolt-on mode. Considering the high number of mills in operation in Brazil, the potential market for the installment of biorefineries is big.

2.2.5. Startups

The terminology *startups* is usually applied to newly founded, innovation companies whose businesses are mainly connected to technology development. In this work, *startups* refer to newly founded companies focused on innovation in the field of biotechnology.

There isn´t a rigid definition of what a startup company really is, the founders of such companies usually point to different characteristics in order to place a company in this category (Robehmed, 2013). However, one point of agreement seems to be that a startup company must be fast growing (Graham, 2012), and once their product is in the market, one way to keep the growth velocity is to make successive innovations over their original product.

Startup biotech companies are so young, innovative and fast growing companies, that their product strategy is usually either present a highly competitive process for an existing product or a production process for a chemical that doesn´t have yet a defined market, adding extra risk to the development.

Because these companies search rapid growth, startups tend to look for partners willing to invest in their technologies during scaleup, to invest in pilot and demo plants to try and get to industrialization as fast as possible, which makes risk management a very important element in this sort of project.

2.2.6. Integration of Sugarcane Mills into Biorefineries: State of the Art

Biorefinery feasibility has been discussed since environmental and non-renewable energy problems awareness rose in the world, especially after the Rio Conference in 1992.

The National Renewable Energy Laboratory, (NREL), published a series of reports investigating the feasibility of a biorefinery and the most promising products and processes. In the report called “Strategic Biorefinery Analysis” in 2002, divided in two volumes, the advantages of biorefinery production versus individual plants and the two bases for biorefineries, corn and sugar cane, were studied. In another report called “Top Value Added Chemicals From Biomass” from 2004, chemical compounds obtained from biomass that have the highest market potential we studied, criteria such as product value, it´s production chain and the available technology were used to classify the chemicals.

Bransby (2008) researched the main challenges for biofuels production from the biomass conversion, biomass logistics and process requirements point of view. Grass biomass would play an important role according to the author, for the first biorefineries, wood biomass was predicted as the feedstock of choice due to its lower costs by energy unit in the present.

Ely (2009) studied the economic and technological aspects that contribute to the biorefinery feasibility, competitiveness factors such as scale and scope were listed and conditions external to the plants such as location were studied. Technological routes were applied to an example where the author pursued to determinate the routes for a biorefinery that yielded successful economic results given the biorefinery location.

Hytönen (2009) presented a method for identification under uncertainties of technologies to be implemented in a forest biorefinery. The objective of the study was to use risk analysis with Monte Carlo simulations to identify the most promising technologies to be installed in a biorefinery, economic results (IRR) were compared and standard deviation was used as measurement of riskiness of each technology, sensitivity analysis helped identify the critical variables of the processes. Technologies studied involved pretreatment of biomass, gasification, production of ethanol, production of acetic acid, and higher alcohols. Sensitivity analysis concluded that the most critical variables of the analysis were: End product prices, fossil fuel prices due to transportation, enzyme cost, electricity and oxygen cost with the added comment that both were relatively certain numbers. The author concluded that in this case the comparison of economic result and risk analysis wouldn´t yield a different rank of technologies when observing IRR, but comments that there are other economic results from a project to be observed such as capital investment.

Bozzell (2010), studied the technical feasibility of biorefineries, divided the implementing objectives into two main branches, energy, accounting for biofuels production such as ethanol, butanol and biodiesel, and economics, accounting for the production of chemicals for application in diverse areas of the chemical industry. According to Bozzell, biofuels, albeit the big volumes, have low market value, reducing the incentive for biorefinery construction, this incentive must come then from chemicals with low volumes but high market values, yielding higher margins for biorefinery projects.

Oliveira (2010) studied the feasibility of biorefineries in Brazil from the perspective of the possible products generated from biomass and the country´s demands, also studied the construction of a greenfield biorefinery based on a sugar and ethanol plant. The technical challenges to integrate a biorefinery to a sugar and ethanol mill, such as energy integration necessary so the lignocellulosic material, used as fuel currently in the mills, can be diverted for chemicals or biofuels production, also the issues about the use of different types of biomass were studied.

Sengupta (2010) studied the integration of bioprocess plants into a chemical complex in the Mississippi river area, analysis were done in light of economic, environmental and sustainability results, for which economic analysis, life cycle analysis (LCA) and other sustainability methods were used. In the integration process, it was possible to reduce the carbon dioxide emission to zero, reducing its impact to global warming, when economis are concerned, it was possible to increase operational profit by over 80% and in the sustainability area the calculated social cost of the plant was reduced in 44%.

The Brazilian Enterprise for Agricultural Research, in its book named *“Biorrefinarias: Cenários e Perspectivas”* (2011), a compilation product of its National Biorefinery Symposium (SNBr), explored the potential of biorefineries in Brazil and lists as the two main production chains in Brazil´s agribusiness the ethanol production from sugar cane and the biodiesel production from soy. This work identifies energy and chemical sectors as the main benefiters from biorefinery development.

Dias (2011) studied an integrated process to produce first generation ethanol from fermentation of sucrose from sugar cane and second generation ethanol, from fermentation of lignocellulosic sugars from bagasse and straw. Different biomass transformation processes were studied and economic analysis were performed for each, the work concluded that two factors were pivotal for the economic success of the processes, one is the reaction duration time that highly affects the capex and the other is catalyst usage, which affects heavily operational expenses.

Mariano (2013) studied the integration of a butanol plant from ABE fermentation of pentoses from lignocellulosic material into a greenfield sugar and ethanol mill project, and compared it to the production of biogas from the same pentoses. Integration of the butanol plant increased the diversity of the mills products with the addition of butanol itself and the by-product acetone, the diversification helped the project achieve internal rates of return around 15%, whereas implementation of biogas production yielded internal rates of return around 11%.

Mariano (2013) also compared the greenfield installation of a biobutanol plant annex to a sugar and ethanol mill with a 50/50 sugar and ethanol mill and concluded that the biobutanol plant helped increase the internal return rate of the project from 13.3% to 14.8%, sensitivity analysis and Monte Carlo simulation were used to define important parameters influencing the economics and the probability of each scenario to reach a minimum 12% IRR, reaching a result for P of 0.99 for a biobutanol plant and 0.8 for a sugar and ethanol mill. The performance was only achieved when biobutanol was produced by an improved microorganism and butanol was sold in the chemical market, with higher value.

Treasure (2014) performed economic and risk analysis on a process to produce ethanol from biomass using dilute acid pretreatment, enzymatic hydrolysis and co-fermentation of the lignocellulosic sugars. A complete process model based on studies done by NREL was done and risk analysis was performed with the @Risk software, the same used in this work. The authors concluded that a 12% return on such project is possible if ethanol prices reach 0.85US$/liter for hardwood feedstock. Variables affecting the most the projects economic results were also identified such as ethanol revenue, biomass cost and composition.

Techno-economic feasibility of biorefineries in its many configurations is a subject of upmost interest in the technical community, biorefineries being the path for biofuels and biochemical feasibility. Adding to the economic analysis, financial risk analysis of the projects have also been studied lately and recognized as an important step in project analysis. In the body of work found in the literature, when the economic and risk analysis of the project is carried out, a great deal of technical development of the process is already under way, simulations, flow sheets, design, capital estimations and reliable process data are already available. Also, when integration of the biofuel or biochemical plant into a biorefinery is studied, the biorefinery is usually studied as a whole, complete venture.

This work intends to add to the body of knowledge by proposing a method of project analysis that can be used in the early stages of a project, when very little technical information is available, and that is flexible enough for analysis of a biorefinery, a plant or even a single technology. Also, the method proposed aims to identify, besides economic parameters such as prices of chemicals and raw material, process parameters that have an important impact in the economic result of the project so it can be used in the technical development planning of the project.

2.3. Project Economic Analysis

In research and development, economic analysis is an important effort in order to assess and evaluate if a project is likely to yield a financial return to the players investing in its development, if the players investing in a technical development of a plant receive a financial return when the plant operates, they will then be able invest in the next technological development and then in the next, and so on. Economic analysis is then an important step in guaranteeing the sustainability of the research and development done in the industry.

Economic analysis can be performed from the very beginning of the project, even with uncertainties; it will already yield important information about the economic feasibility of the project. As the project progresses, economic analysis are updated, becoming a live document reporting the evolution of the project.

2.3.1. Capital Investment Estimation

One of the key items in economic analysis is the capital investment estimation; it is also a source of great uncertainty in early stages of a project. When trying to estimate the required capital investment in an early stage evaluation, there are some procedures or methods that could give out an estimate at an acceptable level of uncertainty.

For an economic analysis project in early stage to be done, a precise estimation of the investment is not possible, nor is necessary, an order of magnitude (in ANSI classification) or Class 5 (in AACE classification) estimation is enough. Order of magnitude or Class 5 estimations have a precision expected to be from 20% to 50%. (Peters, et al., 1991), (Turton, et al., 2012).

2.3.1.1. Preliminary Screening Estimation Methods

In an early stage evaluation, a number of possibilities for capital investment estimation depending on the resources at hand; data history for similar projects could be used if available, or even an educated guess could work depending on the case. One tool that engineers have long been trying to develop and perfect are capital investment estimation methods.

Petley (1997) studied the estimation methods described in the literature and divided them in three groups

- Exponent Estimates: takes data from operational plants, and estimate the cost of the new plant by a ratio between the capacities of the new and the operational plants raised by an exponent.
- Factorial Estimates: when certain cost factors from a plant are multiplied to yield the cost investment of the full plant.
- Functional Unit Estimates: when the number of functional units of the plant and data known in the early stages of a design are used to calculate the investment cost through an equation.

There is a large variety of estimation methods being developed for the last decades, but they are mostly outdated and were mainly developed for petrochemical process, not representing the specifics of biochemical process (Tsagkari, et al., 2015), so extreme caution should be exercised when using such methods.

2.3.1.2. The Process Step Scoring Method

The method chosen for capital estimation in this work is the Proces Step Score, developed by Taylor (1977). Aside from yielding results with acceptable precision for an early stage evaluation (Tsagkari, et al., 2015) (Gerrard, 2001), it has the advantage of including process information into the calculations, meaning it is possible to include process parameters such as solids concentration on hydrolysis or solvent concentration in fermentation in the factors that influence the investment cost. It is a useful feature since one of the objectives of this work is to identify process parameters that are influential in the economic results of the project in order to aid the development plan.

In the Process Step Scoring proposed by Taylor, the production process is divided in processing blocks, normally coincident with reaction or separation steps, and for each step is calculated a complexity score based on throughput, process conditions such as temperature and pressure, and special process characteristics such as safety special measures or tight product specifications. A whole complexity score of the process is calculated and then capital investment is estimated according to the Eq 1. (Tsagkari, et al., 2015).

$$C = 0.121 * \sum_{1}^{n} (1.3)^{S} * Q^{0.39} \qquad \text{Eq 1}$$

Where:

C: Cost of capital investment ($);

N: Number of significant process steps;

S: Complexity score calculated for each step;

Q: Plant capacity (kt/y);

In order to calculate the complexity score for each step, a scale relating the complexity with the process parameters was devised, for each step, the parameters such as throughput, temperature and pressure are used to calculate the complexity according to the scale. Figure 2.10 shows the chart used for the complexity calculation.

The estimation obtained with the process step score represents the inside battery limits investment cost which is the investment required in the actual product manufacturing sections of the plant. The outside battery limits (OSBL) cost is the investment cost demanded by adjacent structures of the plant such as raw material and consumables storage, interconnections with utilities and buildings, OSBL is estimated as a ratio with ISBL, in this work, the ratio between OSBL and ISBL is considered to be 50% (Bray, 2007).

Scoring for complexity of significant process steps

	Score -3	-2	-1	0	1	2	3	4	5	6	7	8	9
Relative throughput (*t/t* product)	0.2	0.35	0.6	1	1.7	3	5	8	14	23	40	67	110
Reaction time in h (reaction, crystallisation, etc)				3	5	9	14	25	42	69	120		
Storage time in weeks				1	2	3	5	8					
Temperature extreme (°C) Min				20	−25	−75	−125						
Temperature extreme (°C) Max					500	1100	1700	2300					
Pressure extreme (atm) Min				1	0.1	0.01							
Pressure extreme (atm) Max					10[a]	50[a]	200	700	1500				
Materials of construction				MS[b]	SS[c], Keebush RLMS[d], EbLMS[e], PVC	ELMS[f] Inconel Nickel Monel PbLMS[g]	Titanium Hastelloy	Precious metals Tantallum					
Multistreaming. No. of streams				1	2	3	5	7	11				

Special conditions:
(a) Explosion, dust, odour or toxicity problems. Score 1 if a major problem.
(b) Reactions in fluid beds. Score 1.
(c) Distilling materials of similar b.pt. Score 1 if b.pt. difference <5°C and Score 2 if <1°C.
(d) Tight specification e.g. Score 1 if distillation is to reduce 'key' component to 10 ppm level.
(e) Film evaporation e.g. in Luwa. Score 1.

Conversion of score to costliness index

Score (S)	−3	−2	−1	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
Costliness index (*I*)	0.4	0.6	0.8	1	1.3	1.7	2.2	2.8	3.7	4.8	6.3	8.1	10.6	14	18	23	30	39	51	66

[a]For liquid phase reactions only. All others score = 0. [b]MS = Mild steel. [c]SS = Stainless steel. [d]RLMS = Rubber lined mild steel. [e]EbLMS = Ebonite lined mild steel. [f]ELMS = Enamel lined mild steel. [g]PbLMS = Lead lined mild steel.

Figure 2.10 The Scoring of the Process Step Score Method (Taylor, 1977).

2.3.2. Operational Costs

Besides the capital cost of the project, its operational costs are also calculated in order to perform economic analysis, the operational costs are divided into two major groups, variable costs and fixed costs.

Variable costs are all the costs that are production dependent, the more the plant produces of its product, the higher these costs are, on the other hand, variable costs are constant when calculated as specific costs, i.e. cost per unit of production. Variable costs include raw material, consumables, and utilities costs and are calculated with the aid of the mass and energy balance.

Fixed costs are all the costs that are independent of the production, these costs are factored even if the plant is non-operational. Contrary to variable costs, fixed costs are not constant when calculated as specific costs, and tend to be lower the higher the production, Fixed costs include labor, overheads, maintenance and site costs. Maintenance costs are usually estimated as a percentage of the inside battery limits (ISBL) investment cost, labor is calculated according to geographic labor compensation references, overheads represent costs with administrative workers and are calculated as a percentage of labor work and site costs are usually estimated by using references from existing plants.

2.3.3. Economic Analysis

There are a few project economic metrics that can be calculated in order to evaluate the capacity of a project to provide financial return to the investor, the internal rate of return (IRR), net present value (NPV) or the ratio between the NPV and the capital invested can be used as metrics.

In this work, the NPV is chosen as the economic output for project evaluation, the net present value represents the value of a cash flow, regressed to the present day using a determined discount rate. When the NPV is zero, the internal rate of return of the project equals the determined discount rate. A discount rate of 11% was used in the risk analysis, and the probability of the project achieving an NPV greater than zero (and thus a rate of return greater than 11%) was determined.

It is not the intention of this work to prove the feasibility of the projects evaluated but to present a methodology for evaluation, so no further effort was made in determining the correct rate of return for the NPV calculation, such effort would involve evaluating the country risk, capital market rates of return and origin of the investment resources used in the project.

2.4. Project Risk Analysis

In this work, financial risk analysis of the project is used to determine the probability of the project achieving a desired economic result and also determining the barriers and leverages of the project in order to aid the development plan.

2.4.1. Motivation Behind Risk Analysis;

Virtually every enterprise or group interested in investing funds in a project makes some type of assessment in order to have some assurance over its economic results. Hertz and Thomas (1983) described the evolution of such analysis; Figure 2.11 shows a simple project assessment.

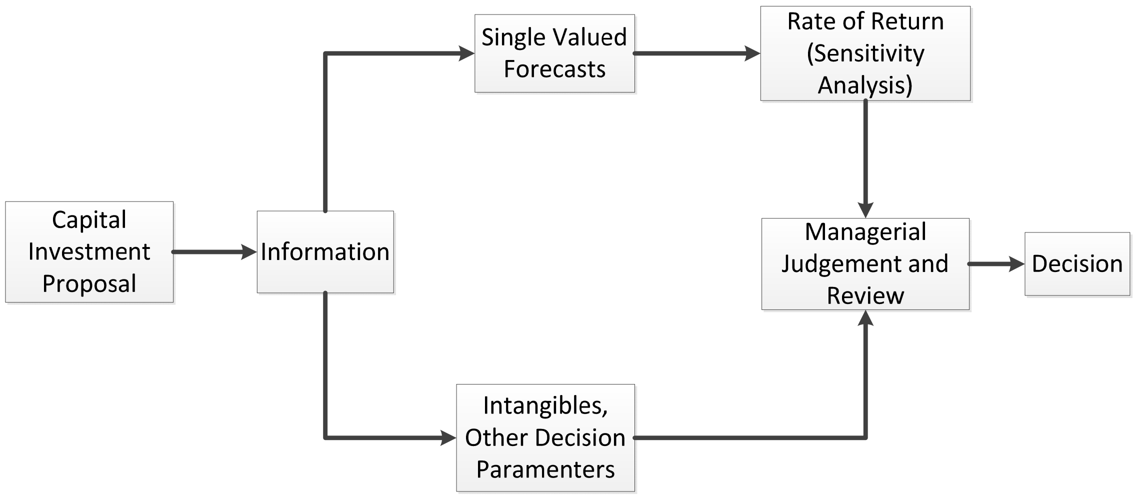


Figure 2.11 Basic Project Appraisal – adapted from Hertz (1983).

This assessment is based on static values for the variables, and in some cases a sensitivity analysis is done to evaluate critical aspects of the project and get a feeling of how easily the economic results could turn undesirable.

The risk analysis assessment shown in Figure 2.12 introduces the distributions for decision variables and the method for calculation of the distribution for the output variables such as NPV, IRR and payback. The distributions of the variables add an extra dimension over the sensitivity analysis, with the indication of a possible range and the values that are most probable to happen whereas in the sensitivity analysis the variables range in fixed amounts to explicit the relationship between the varying inputs and the output.

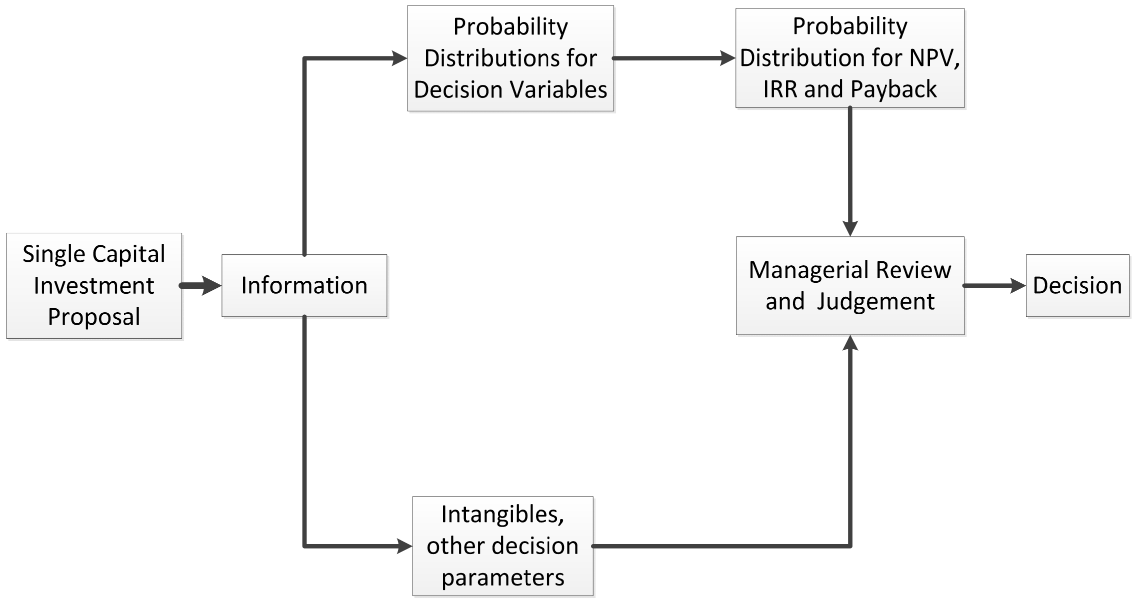


Figure 2.12 The Risk Analysis Process – Adapted from Hertz (1983).

2.4.2. Monte Carlo Simulation in Risk Analysis;

A Monte Carlo type simulation is used in the risk analysis in order to run the mass and energy balances and the economic model a great number of times using the probability distributions defined for the inputs in order to obtain the probability distributions of the appointed results and the correlations between the variables and the results.

Monte Carlo simulation is the method used by risk analysis software such as @Risk and Crystal Ball, so it is widely used for risk analysis in every area of expertise. Monte Carlo is mathematical method used for modelling stochastic systems, a stochastic system is one that is heavily influenced by random variables thus not being fully describable by deterministic modelling methods. Economic analysis in the initial stages of projects of chemical plants present a number of uncertainties in the variables involved: raw material and product prices, process yields that could evolve during development, etc. Because of such uncertainties, techno-economic analysis of chemical plants can be modelled as a stochastic system and thus, be assessed via a Monte Carlo simulation.

More on the functioning of the Monte Carlo simulation in the @Risk software and Excel spreadsheets can be found in section 3.4

2.4.3. Assigning Distributions to Inputs;

Assigning the distributions to the inputs is an important step in the risk analysis. In an ideal situation, it would be possible to access historical data for all the inputs, statistically define the distributions and use it in the risk analysis, in the analysis of early stage projects, there might be some variables that have history records and can have its distributions calculated, prices for instance, but that might be very rare for technical data.

Not having historical data on a variable does not keep the evaluator from assigning a distribution to that variable, but it should be done with care. If that variable proves to be influential in the economic results, then it is a good procedure for the estimator to run a second round of analysis after refining the variable´s distribution. Except in a few cases that will be discussed in the biobutanol project (enzyme price), all variables without historical data assessment should either be assigned to a normal distribution or a triangular distribution around the known value. The normal distribution should be used when the variation is symmetric to the best knowledge of the estimator and standard deviation should be adjusted to fit the range found to be adequate. Triangular distribution can be used when the variation is known not to be symmetrical or when there is a limitation, for instance, if the variable is a chemical conversion, so it can´t be higher than 100%.

A tree decision tool for choice of distribution types is shown in Figure 2.14.

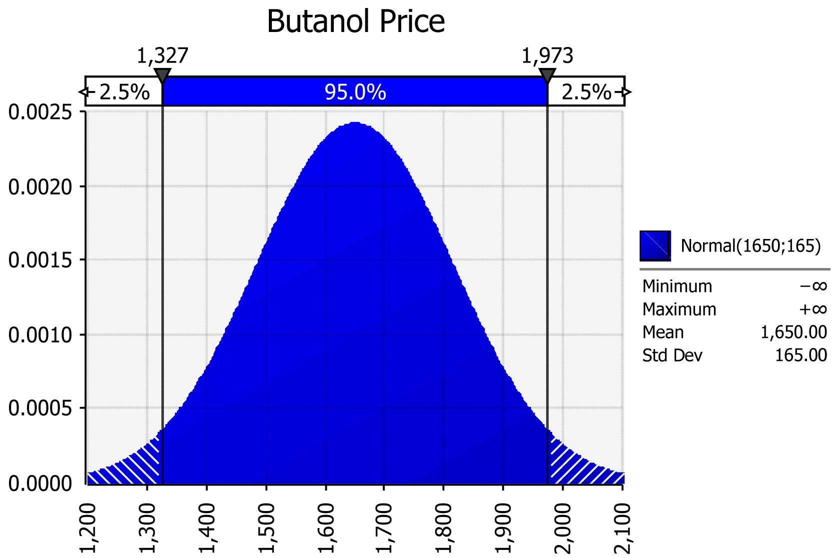


Figure 2.13 Generic Example of Normal Variation Assigned to a Variable -Butanol Price-. (Graph Made with @Risk)

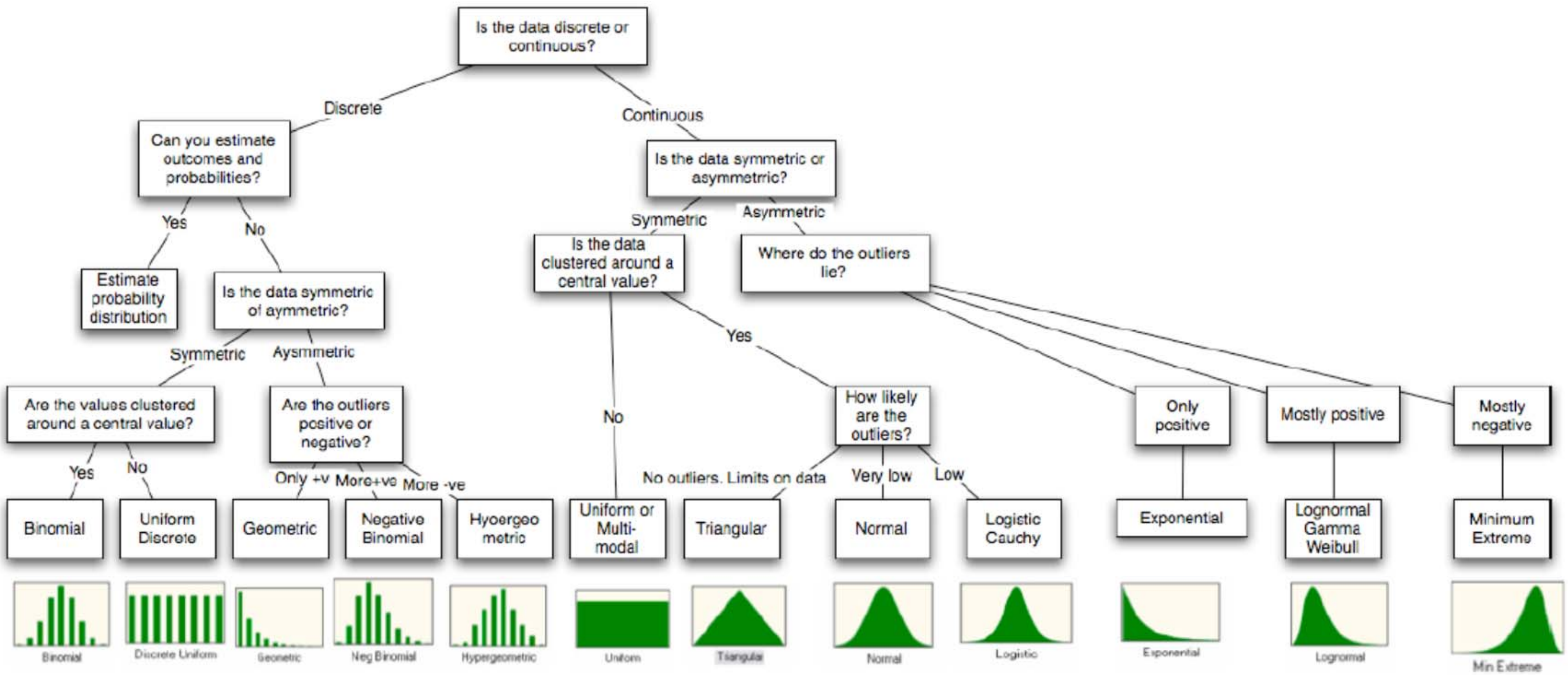


Figure 2.14 Distribution Fit Tree (Damodaran, 2006)

2.4.4. Analyzing the Results;

To assess the risk analysis or to answer the questions that risk analysis should address, there is a number of different results or graphs that can be used. The first question to be answered, is concerned with the probability of the project yielding a desired economic performance, or the probability of the project yielding a bad result, and it can be answered by the analysis of the resulting distribution graph of the economic indexes, namely IRR and NPV, and also capital investment, variable costs, full manufacturing costs, etc.

It is also possible to use risk analysis to increase the technical comprehension on the project, which means calculating the distributions not only for the economic results but for the mass and energy balances results as well as any calculation done in the model. With this, steam consumptions, plant efficiencies, equipment sizes, virtually any result can be expressed as distributions. For example, the project team can estimate the probability of the fermenters of the plant being too large to be built in the manufacturer and transported to site.

Figure 2.15 shows an illustrative example of a resulting distribution, it is possible to see in the graph two main information, the first being the form of the distribution histogram itself indicating the results that are most probable to happen, second is the bar that indicates with 95% confidence what is the range of this output. In the software @Risk, it is possible to manipulate this graph in order to obtain the probability of a given result happening, for instance IRR>20% or NPV>0, this feature will be used in the analysis of the biobutanol and muconic acid cases.

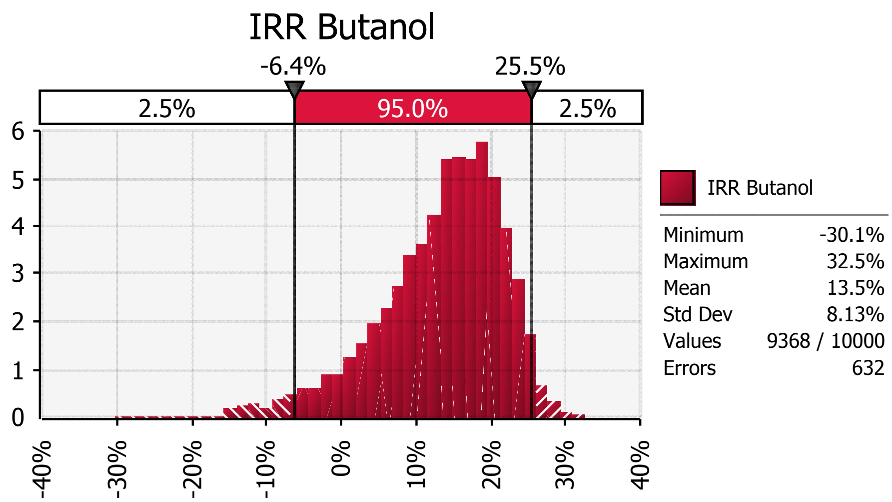


Figure 2.15 Generic Example of Calulated Distribution in @Risk

After analyzing the distribution of a given output, it is possible to answer the second question directed at risk analysis, identifying the barriers and leverages of the project. This type of analysis is useful not only to drive a decision, but also to help defining the path of development in bench or pilot scale.

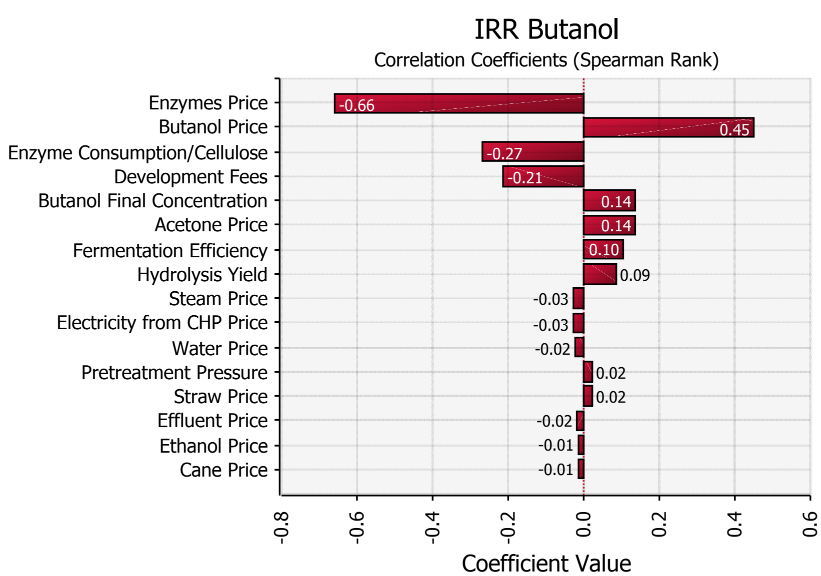


Figure 2.16 Generic Example of Graph Displaying Influences on a Variable

Figure 2.16 shows an illustrative example of a graph showing the variables that have the biggest correlation with the target output. There is also two main information to be drawn from this graph, the first is the correlation itself, that can be seen by the size of the bars and the numbers on each one, the second information is the direct or reverse correlation between the variable and the output, that can be seen by the orientation of the bar, to the left meaning an inverse correlation variable, to right, a direct correlation variable.

3. CHAPTER 3: TOOLS AND METHODS

3.1. General Method

In order to build a dossier that will make it possible for the stakeholders of the project to make the best possible decision, a series of tools and methods will be used to raise pertinent questions, understand fully all aspects and uncertainties of the project and predict its possible scenarios and outcomes.

Figure 3.1 shows the general methodology for the analysis of an integration project in early stages. The first step is to gather information on the process to be studied; this information can come from many sources: patents, academic work, partners that are technology developers. Building a simplified mass and energy balance is the following step in order to obtain an economic analysis, a simplified mass and energy balance means it should be based on a block diagram; mass balance of general process steps is made instead of equipment.

After the mass and energy balance is done, consumption of raw materials, other consumables and utilities is calculated for variable cost calculation and fixed cost is estimated.

Capital investment can be estimated by a number of ways, or in the case of very fast analysis it can be considered as a variable itself, based on gathered information. In this work the method used for capital investment estimation is the Step Score method that is detailed in sections 2.3.1.2 and 3.3. Economic analysis is run and the main project metrics are calculated, e.g., NPV, a number of different metrics can be used depending on the project.

In order to perform the project´s risk analysis, the main variables are identified and distributions are assigned to them, the logic of assigning distributions to variables is explained in section 2.4.3. With distributions defined, a Monte Carlo simulation is run, in it, five to ten thousand calculations of the mass and energy balance and the economic analysis are performed, the input variations obeying the distributions previously defined.

The result of the Monte Carlo simulation is that the economic metrics searched and the mass and energy balance results can also be portrayed as distributions, with such distributions it is possible to try and identify the probability of a desired or undesired event to happen, for example, the probability of the NPV being greater than zero. Another important result coming from the Monte Carlo simulation is that, having performed many calculations with varying inputs, it is possible to calculate the correlation between the inputs and the economic and technical results of the simulation, these correlations are important to help further improve the risk analysis, by better defining the distributions of the most important inputs, and help project development by identifying the factors that impact the most the project´s results.

A report with the distributions of the main project metrics and the correlations between these and the project´s inputs will drive the project team to two main decisions, first, if the projects results and risk profile match the investment policy of the group/company and if the project should continue, what are the areas in which to invest the most R&D resources.

Flow Diagram	Tools / Information Sources	Notes
Process Information	• Patents. • Scientific Papers; • Technical Information; • Partnerships;	• Data; • Process Parameters; • Rules of Thumb;
Mass and Energy Balances	Excel Spreadsheet	
Economic Analysis	• Excel Spreadsheet; • Step Scoring	• Variable Cost; • Fixed Cost; • CAPEX; • NPV; • IRR;
Risk Analysis Main Variables Distributions Definiion Analysis Risk Analysis Approval	• @Risk • Excel Spreadsheet	• Monte Carlo Simulation • Sensitivity Analysis
Comparison to investment policy/ Decision		• Result Distributions

Figure 3.1 General Methodology and Tools Employed in this Work

In this work, three case studies will be developed, in them; it is shown that the methodology presented in this work could be applied in projects with very different scopes. In the first case, presented in Chapter 4 a biorefinery integration of a biobutanol plant with a sugarcane mill is studied, economics and risk analysis are run taking into account the feasibility of both the biobutanol plant and the biorefinery as a whole. By studing both the isolated biobutanol plant and the biorefinery, the objective is to evaluate first if the biobutanol process presents acceptable economic results and if the transformation from a sugarcane mill to a sugar cane plus biobutanol plant produces acceptable economic results, because the introduction of a biobutanol process have some impacts in the sugarcane mill production: the first is the reduction of exported electricity due to the energy requirement of the new annexed plant and the second is a reduction in the ethanol production, since some molasses could also used in the biobutanol fermentation as an additive because of the salts and nutrients contained in it.

In the second case, presented in Chapter 5 a muconic acid process is evaluated, this case validates the methodology of analysis of a process with very low quantity of information. In the first case, (ABE fermentation), although the analysis is done at early stages level of a project, it is possible to build a fairly detailed mass and energy balance from literature information since it is a well-known process. In this case the only source of process information for muconic acid manufacturing is a patent filed by the company Myriant (2013) and it is used as basis for the construction of a mass and energy balance, process information not contained in the patent were filled by rule of thumb process design. The process to produce the lignocellulosic sugars for fermentation was based in the work done by Bereche (2011), the same considered for the biobutanol case. Economic and risk analysis were performed to evaluate the feasibility of the muconic acid process.

In the third case, presented in Chapter 6 an analysis of the lignocellulosic sugars production process is presented. The objective of this case is to analyze a part of the process as if it were a complete plant by treating the sugars produced as a valuable product; its cost and minimum price are calculated. With the minimum price of the sugar, that is, the minimum transfer value of the sugar to a plant that would produce any chemical from it that would yield an acceptable return over the investment on producing the sugars, it is possible to try and predict what type of chemicals could be produced from this sugar with economic feasibility. Calculating across the whole range of yields possible in processes that would transform sugars into chemicals, from fermentation yields to other chemical reaction yields and using rule of thumb metrics to try to predict the cost of production of such chemicals, an analysis is done to verify which chemical segments (fuels, solvents, specialties, etc.) could be fulfilled by these chemicals. Process information for the lignocellulosic sugars manufacturing process is based on the work by Bereche (2011). This analysis assumes that market segments for chemicals usually have a typical range of production costs, for instance, fuels must be produced with costs under US$1/kg.

With the three cases, risk analysis is showcased in three different situations, showing that the method can be applied to a big number of projects in early stages or even as a tool to define global R&D strategies. It is shown that the methodology can be applied to a broad system such as a biorefinery, to a chemical manufacturing plant such as the muconic acid plant and also to a single technology to assess its value proposition such as the lignocellulosic sugars via enzymatic hydrolysis technology. A schematic of the scope of the three analyses is shown in Figure 3.2.

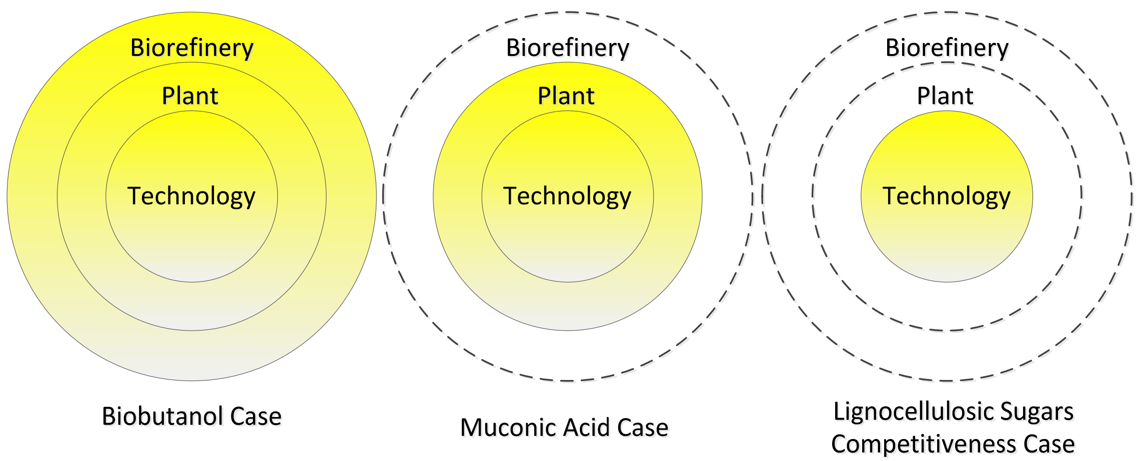


Figure 3.2 Schematic of the Scope of the Three Analyses Presented in this work.

3.2. Mass and Energy Balances

The first step to be built and the core of this analysis is the mass and energy balance of a sugar and ethanol mill and a biobutanol plant using the ABE fermentation technology. This step will be built using the tool Microsoft Excel spreadsheet software. Its main characteristic should be simplicity, in early stages of the project the uncertainties are too big to support the use of complex mathematical modeling, there is usually no hard data on the process to support deep process modeling for instance, also, a mass and energy balance with simpler calculations will make it more accessible for the project team to understand all the variables influencing the results. Not using complex models for kinetics and separation process will surely have an impact on the precision of the predictions made, this could always be introduced later in the project, when information availability is greater and the benefits will be clearer and thus worthy of the great man-hour necessary on this effort.

The mass and energy balance will be divided in two main sections, the sugar and ethanol mill and the Biobutanol plant, and each one will be subdivided in the following sections:

- Sugar and Ethanol Mill;
    - Grinding;
    - Juice Treatment;
    - Sugar Plant;
    - Fermentation;
    - Distillation;
    - Combined Heat and Power;
- Biobutanol Plant;
    - Biomass Pretreatment and Hydrolysis;
    - Feedstock Treatment;
    - Sugar Fermentation;
    - Distillation;
    - Utilities;

Numbers such as specific consumptions (steam, electricity, chemicals) will be used as estimated by literature and common knowledge; these factors will be target of sensitivity analysis to determine the influence on each one on the economics of the project.

The mass and energy balances will be performed for two different scenarios: on the first, a biobutanol plant will be annexed to a sugar and ethanol mill, using bagasse, straw and molasses as feedstock and using the same utilities as the mill, i.e. steam and electricity produced from bagasse and straw burning. On the second scenario, that will compete with the first, a mill simple expansion will be calculated, with an increased input of sugar cane and increased productions of sugar, ethanol and electricity for the grid.

The results expected specifically from the mass and energy balance are the flows of the main streams of the process, which will be used for capital investment estimation and the consumption of raw material, chemicals and utilities that will be used for operation expenses calculations.

3.3. Economic Analysis

The results of the mass and energy balances will feed an Economic Model in which the cost of operation and investment of the project will be calculated, and then the profitability of the project will be determined by the Internal Rate of Return, Net Present Value among other economic criteria.

The operations cost will be calculated using raw material consumption and costs, consumables and utilities costs will be calculated with aid of mass and energy balances, also, fixed costs will be estimated for a sugar and ethanol mill located in Brazil countryside.

Capital investment for both the biobutanol plant and the mill modifications will be estimated using an early project capital investment estimation methodology. This methodology estimates the capital cost of a plant by dividing it in process sections and estimating the complexity of such sections, the complexity of each section is equivalent to its contribution on the total investment (Taylor, 1977) more details of this methodology will be explored in Chapter 5. In such early stages of a project, there isn´t a demand for a highly precise capital investment estimation, projects in early stages have high uncertainties and a number of unknown factors which makes it void to put too much effort in estimating capital investment with a high degree of precision.

A fee for technology development will be considered, in almost all new technology developments, a technology company licenses the use of its proprietary technology, being it a new process, or a catalyst or a microorganism in exchange of a fee to be paid by the producer. So a technology license fee should be considered as an expense in the economics of the project.

The full manufacturing cost of production will be estimated, a cash flow diagram will be built with a business plan which will yield return rates, present values, break even times, etc. These are the economic metrics expected from this analysis, and that will be target of the next step in project evaluation, risk analysis.

3.4. Risk Analysis

Risk analysis is the final step in this work´s project analysis. Its main objective is to primarily estimate the probability of a project achieving the return on investment calculated in the economic analysis, also, risk analysis is an important decision making tool because it allows to estimate the odds of a project yielding a weak result, that could put the business at risk. The risk analysis adds a new dimension to the project evaluation as it gives a risk information together with an economic information.

The biggest problem in defining a go/no go on a project is not calculating the return based on its premises, but the validity of the premises themselves; a handful of premises with often big uncertainties can yield a project with uncertainties of critical proportions (Hertz, 1979), hence the necessity of the risk analysis to stablish, with a higher degree of confidence, the economic feasibility of a project. Even after approval of project feasibility by the stakeholders, risk analysis still plays a crucial role identifying and finding ways to mitigate factors that have the highest probability of affecting negatively the project outcome. To perform the risk analysis, sensitivity analysis will be used to identify the variables that affect the most the economic results of the project and Monte Carlo simulations will be used to calculate the probability of the project achieving a given economic result. After the feasibility of the project and its risks are determined, the project´s killers and leverages will be analyzed individually to design a path forward to mitigate risks and leverage the most important aspects of the process that can help increase project results.

Sensitivity analysis will be carried out through tornado graphs, which shows the variation of the result of a system according to the variation of each of the chosen inputs individually. The intention is to show which one of the variables chosen (yields, prices, efficiencies, etc.) have significant impact on the final result of the project (Return Rates, Present Values, Investment Estimations, etc.).

A Monte Carlo simulation will be carried out with the objective of calculating the probability that the economics of the project will yield the expected results. Probability distributions will be assigned to each variable according to general market information, technical information and historical data when available. All distributions together will contribute to build the scenarios with the highest chance of happening. This method is named after the famous casino in Monaco, and relies on random number generation and probability estimations to generate as much feasible scenarios as necessary. This method is used particularly to predict and analyze so called chaotic systems, for instance those with too many variables which would be too hard to describe in a deterministic mathematical model. The Monte Carlo method will be carried out through the usage of the @Risk software distributed by Palisade.

The @Risk software runs inside an Excel spreadsheet, once the software is activated, the user selects the variables that should take part in the risk analysis, to each variable a range of variation and a type of distribution should be selected, some authors who work with risk analysis using Monte Carlo simulation give a guide to choose probability distribution curves for the variables, this should be discussed in more depth in Chapter 6. The outputs of the analysis are also selected and should be the main process and economic results of the process. After setting the variables and the results, the number of iterations on the Monte Carlo run is selected and the analysis can be started. A Monte Carlo run is initiated and a number of scenarios are calculated to the variations and distributions defined, meaning that all the inputs selected will vary according to the probability distributions.

The Monte Carlo run yields a number of different results to be analyzed, the first type of results are the probability curves of items defined as output, process indicators such as energy, water, chemicals and raw material consumptions, capital expenses estimate, operational expenses estimates, economic indicators such as NPV and IRR. With these probability curves, it’s possible to predict with the desired amount of confidence the range of the result; the range gives the opportunity to analyze the project from a optimistic view or a pessimistic view, giving thus way to the risk analysis. An example of a probability curve produced by the Monte Carlo simulation on @Risk software is shown in Figure 3.3.

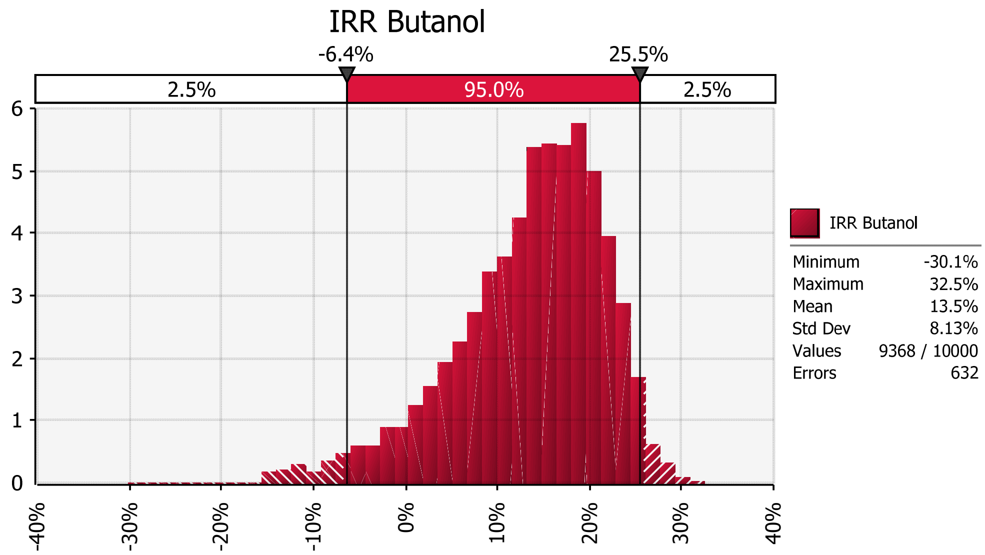


Figure 3.3 Example of a Generic Probability Distribution Generated by @Risk

The second type of results are the correlation graphs, which are presented in a tornado fashion, similar to a sensitivity analysis, but in this case the variables that affect the item being analyzed are ranked considering its Pearson correlation factor from the highest to the lowest. The size of the bar is proportional to the correlation and the orientation of the bar is used as an indication of the variable being directly or inversely correlated to the item, a bar that is positioned to the left indicates an inversely correlated variable, a bar positioned to the right indicates a directly correlated variable. An example of a correlation graph is shown in Figure 3.4.

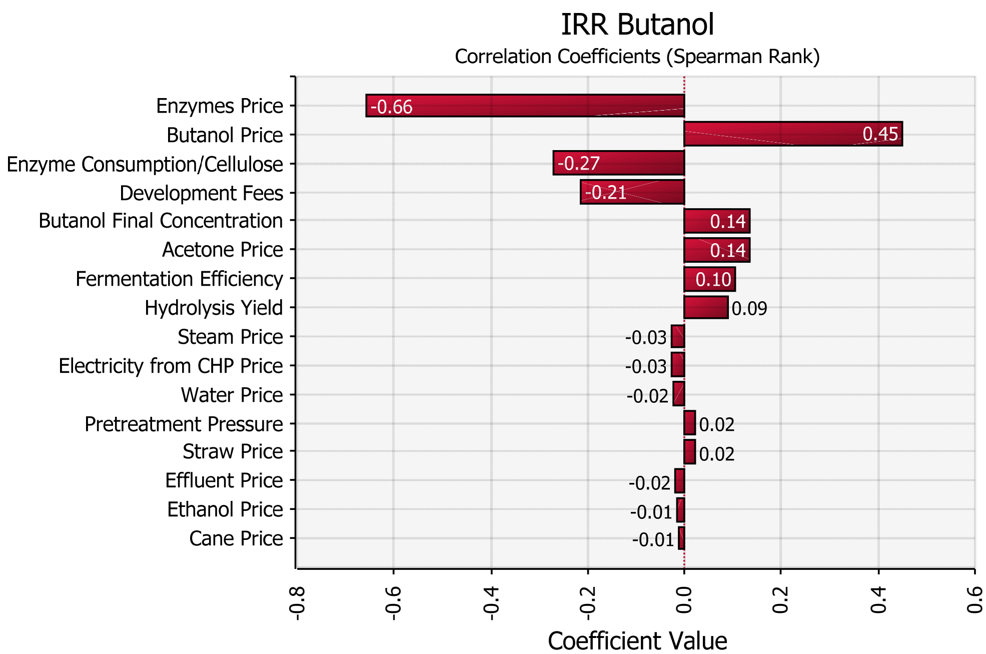


Figure 3.4 Example of a Generic Correlation Graph Generated by @Risk

It is possible also to correlate two items being analyzed, for example, IRR and capital investment by building a graph with all the iteration results produced by the Monte Carlo simulation. In this graph is possible to identify the correlation between both items by the format of the cloud of results formed, a more elliptical form means a higher correlation and a more round shape means a smaller correlation, also, it´s possible to identify if the items are directly or inversely correlated. An example of a cloud graph is shown in Figure 3.5.

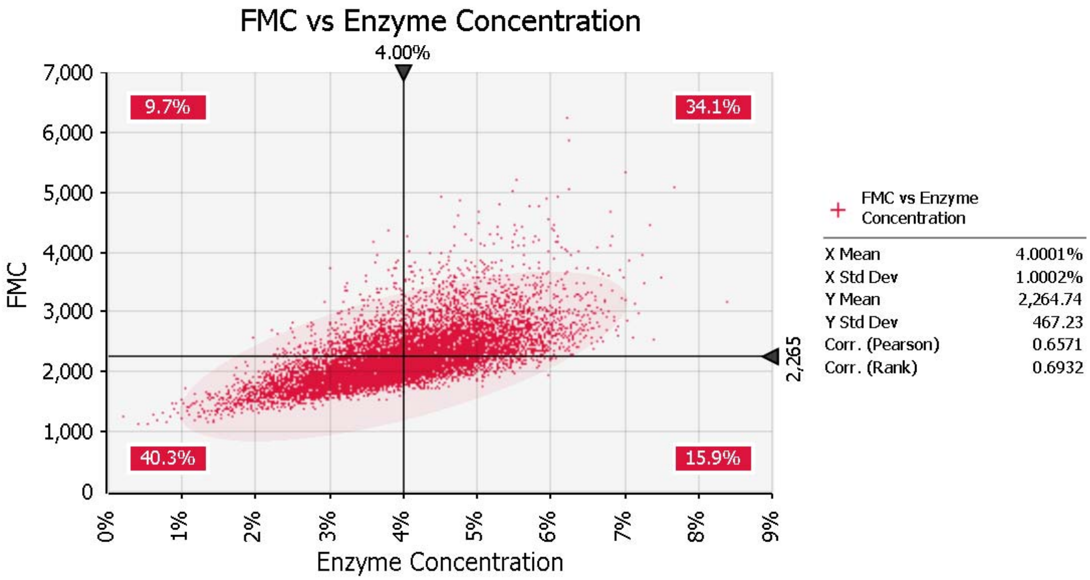


Figure 3.5 Cloud Graph Generated by @Risk

When comparing two different projects in order to define investments, it is common to put side by side the economic results of different alternatives. Comparing just the mean economic result derived from the premises adopted yields an incomplete set of information for the decision makers. In projects such as the object of study of this work, the uncertainties around the premises are high, and, as already stated before, even in projects where premises uncertainties are low, the sum of the uncertainties of all the premises yield a project overall uncertainty that is important. The risk analysis is done with the intent of not only comparing economic results between scenarios but to compare level of project risks.

The expected results from the risk analysis should be a series of probability density curves for the most important economic indicators of the projects. The probability density curves should show as result the probability of each economic result to actually happen, these results will be compared to project approval policies that should define which results and which risks are acceptable in a project such as production of biobutanol through ABE fermentation. The results must also be compared among projects. These factors combined will determine the feasibility of the project, its killers and leverages.

4. CHAPTER 4: BASE CASE I DEVELOPMENT: BIOBUTANOL PROCESS

4.1. General View

The biobutanol manufacturing process to be studied here is the ABE fermentation, in which Butanol, Acetone and Ethanol are produced through fermentation of sugars. In this case, the sugars will be extracted from lignocellulosic feedstock.

The biomass to be treated will be either bagasse or sugar cane straw, depending on availability of feedstock. The sugars will be extracted in two stages, in the first, called pretreatment; the biomass is heated in aqueous solution to temperatures that can range from 130 to 200°C in the so called hydrothermal pretreatment. The pretreatment can also be carried out with the aid of acid, in a technology named Dilute Acid Pretreatment (in both cases the aim of the pretreatment is to extract the sugars from the portion of the biomass called hemicellulose, this fraction of biomass yields mainly xylose, a sugar containing five carbon atoms). In the second stage, the six carbon sugars (glucose) originated in the cellulose, are extracted via enzymatic hydrolysis, which is carried out at mild temperatures and atmospheric pressure for the enzyme to work properly. The enzymatic hydrolysis is considered a bioprocess as much as the fermentation, and, in the same fashion, it needs big residence times to achieve competitive yields. A solid-liquid process step is then used for the separation of the hydrolysate containing the extracted sugars and the remaining lignocellulosic solids containing mainly lignin and residual cellulose and hemicellulose.

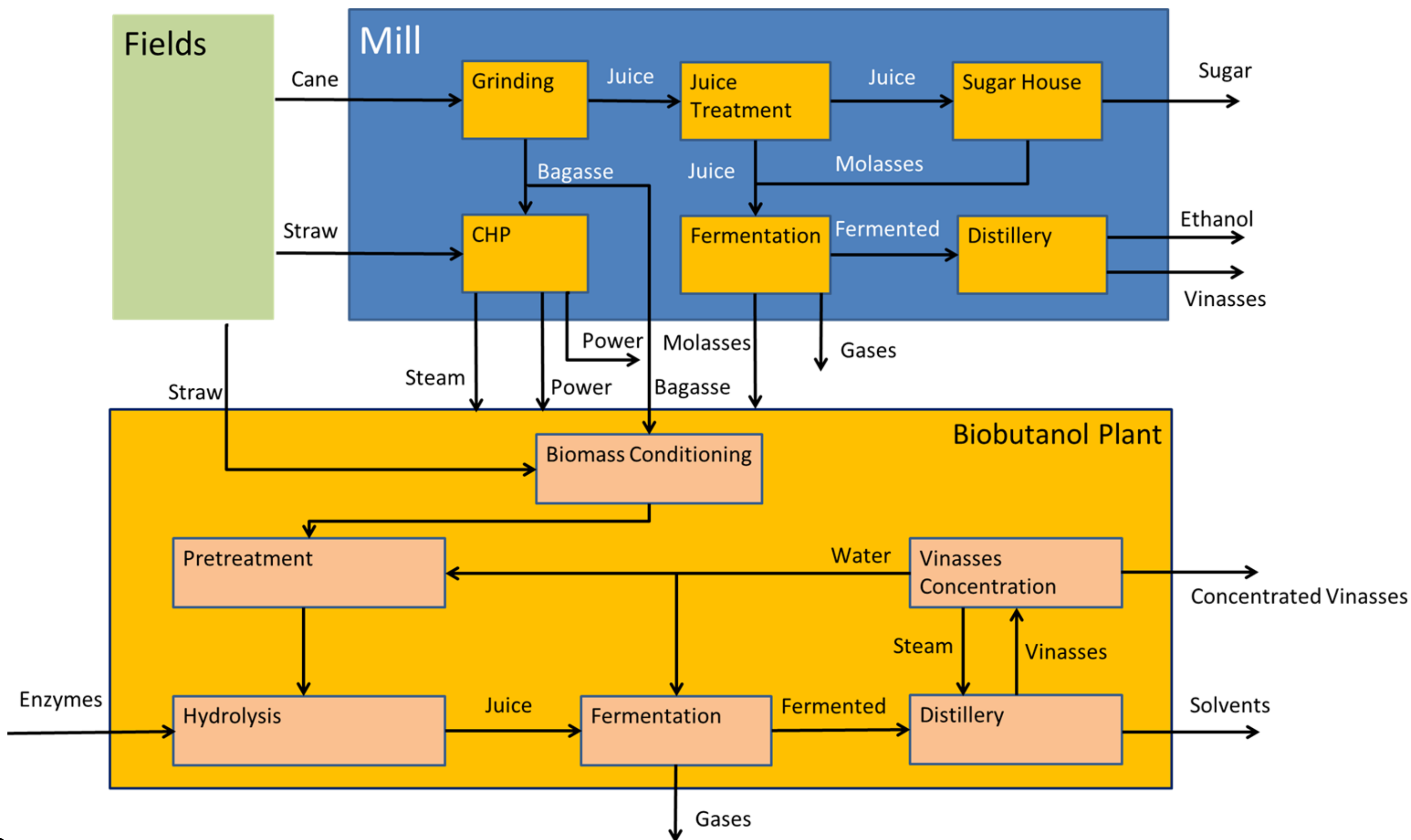
After the separation, the hydrolysate goes through a preparation process to make it suitable for fermentation. For the separation of fine solids remaining in the juice centrifugation, further filtration can be used. During the pretreatment and hydrolysis, a number of chemicals can be generated that act as inhibitors to the fermentation process, so a few detoxification strategies can be used to eliminate these inhibitors such as ion exchange resins, active charcoal, liming and dosage of enzymes such as laccase (Chandel, et al., 2012). A sterilization step is also needed to avoid contamination of the fermentation with external microorganisms; sterilization is carried out through heating of the hydrolysate.

The most common microorganism to be used in the ABE fermentation is the *Clostridium acetobutyllicum* bacteria. This type of fermentation usually yields butanol, acetone and ethanol in different ratios depending on the microorganism. Other parameters are fermentation temperature and tolerance to butanol, which will determine the final concentration of butanol in the fermentation and consequentially the sizes of the fermenters and energy consumption in the process downstream.

Downstream the ABE fermentation the separation process generally considered is distillation as a set of columns in series, where the first column aim to strip the fermentation beer from the solvents and the subsequent columns separate acetone, ethanol and butanol, respectively. Due to the heterogeneous azeotrope formed by butanol and water, decanters are used after the stripping column and in the final separation of butanol and water to make it possible to achieve the targeted purity. Other separation processes that have been studied are membranes, and zeolite pressure swing adsorption.

In this project a butanol plant installed annex to a mill will be considered, where both raw materials and utilities are available for purchase from the mill, eliminating transport costs and the need of a combined heat and power system dedicated to the butanol plant. Steam and electricity needs will be analyzed and must meet both the mill and butanol plant needs for this project to be technically and economically feasible.

The Figure 4.1 shows a block diagram of the integration between a sugar and ethanol mill and a biobutanol plant, this is the configuration considered in this work.



B

Figure 4.1 A Biobutanol Plant Annex to a Mill Simplified Block Diagram

4.1.1. ABE History and Development Perspective

Although biobutanol draws today much interest as a green solvent or fuel, acetone was the product that originally drove the development of the ABE fermentation. Acetone is one of the main ingredients used in the production of cordite, an explosive used in ammunition. The ABE fermentation process was developed before World War I by Chaim Weizmann, who later would become the first president of Israel. Before Weizmann´s development, Acetone was produced from wood, after the ABE fermentation development, plants were built in Europe and India using corn and rice starch as feedstock (van der Merwe, 2010).

Until the end of the first WW war in 1918 there wasn´t much interest in butanol, so the technology was close to be abandoned, but interest rose as butanol became an important ingredient in solvents for the growing industrial activity after the war, which boosted the construction of ABE plants throughout the world. Fermentation was the dominant route to produce butanol until the middle of the century, when petrochemical routes were developed becoming economically attractive.

The petrochemical routes for the production of butanol include the OXO process using propylene, carbon monoxide and hydrogen and the aldol condensation of acetaldehyde. Recently, concerns about the availability of oil in the future and its environmental impacts revived the interest in biobutanol production from ABE fermentation; generating a great quantity of work both in the academic environment and by enterprises seeking to produce butanol from cheap, renewable sources.

Improvements on microorganisms and fermentation process have also been studied to increase ABE fermentation yield and feasibility, e.g. chemical mutagenesis for improved performance, specific genetic manipulation or a combination of the two techniques (Green, 2011). On the process side, companies (e.g. Cobalt Technologies, Green Biologics, etc.) have studied improvements to fermentation such as immobilization of microorganisms or continuous withdrawal of solvent from fermentation media.

4.1.2. Butanol as a Product

N-butanol is an alcohol, a clear, neutral liquid with a characteristic odor, it is miscible with almost all solvents: alcohols, aldehydes, ketones, ethers, glycols, aromatic and aliphatic hydrocarbons (BASF, 2008). It´s miscibility with water is restricted though, producing a heterogeneous azeotrope.

In the chemicals market, more than half of the butanol production is used as solvent for coatings (BASF, 2008), other applications include the production of glycol ethers, plasticizers, solvents for dye paints and printing inks and extractant in the pharmaceutical industry.

The application of n-butanol that has sparked the interest in studies of ABE fermentations to produce biobutanol from renewable sources is fuel. As a liquid fuel, n-butanol has several advantages against its competitors: an energy content 30% higher than ethanol, a low vapor pressure (six times less evaporative than ethanol and thirteen times less evaporative than gasoline) and it also fits the existing infrastructure due to its properties (Green, 2011). Engines working on gasoline can easily use n-butanol without any modification, as already proven in US when a car fueled by butanol alone drove from California to Ohio and back (Brekke, 2007). Also n- butanol is more hydrophobic than ethanol, i.e. it has a higher tendency to repel water and is more suitable for transportation in the same pipes as gasoline, making it possible to use the gasoline infrastructure for distribution.

4.1.3. Feedstock

The fermentation process to produce butanol was developed to use rice and corn starch as feedstock, sucrose from sugar cane or sugar beets can also be used, but interest today is drawn to the possibility of producing chemicals such as butanol from feedstocks that do not compete with food supply and can also be considered as waste. Using waste as a feedstock to produce valuable chemicals has two main drives, economic, since waste should have a very low (or no) price, and environmental, since the chemical produced would not only have the benefit of coming from a renewable raw material, but would also avoid the generation or accumulation of a waste.

In this work, cane bagasse is considered as feedstock, bagasse is not considered today a waste, it is used as fuel for both the energy demands of the site and for energy exporting to the grid. Sugar cane straw or trash, on the other hand, is currently considered a waste, it is a byproduct of sugar cane production and yields the same amount of dry biomass as bagasse. Cane straw plays an important role in the maintenance of the field, keeping it from losing water after harvest, but not the total amount of straw produced should be used for this objective, if too much straw is left on the field, accumulation of rotting organic matter and infestations can damage the next harvests.

Sugar cane bagasse can be used as feedstock for the production of n-butanol and the reduction in the availability of fuel to boilers can be compensated by cane straw. The main motive for this decision is that bagasse tends to be easier to work as raw material for a number of reasons: it has more moisture than straw, which helps water balance since a considerable amount of water is carried into the process by the raw material, reducing the need for process water intake, the milling process for production of cane juice has a positive side effect of washing the bagasse and reducing its size, which helps processing in the pretreatment and hydrolysis steps.

The use of straw for fuel in boilers designed for burning bagasse also presents a few technical issues such as cleaning, chopping and feeding of straw into the boiler, but this work considers that these issues would be easier to address in the context of the mill´s boilers than in the pretreatment and hydrolysis reactors.

4.1.4. N-Butanol production process

The process considered for economic and risk analysis in this dissertation produces n-butanol from the raw material bagasse by first breaking down the biomass into its three main fractions and then using bacterial fermentation to transform two of them (cellulose and hemicellulose) into solvents.

The technology chosen to break biomass into its fractions was hydrothermal pretreatment followed by enzymatic hydrolysis, the fermentation step is carried out in a batch system and separation of the solvents is done through distillation. This are the most commonly known technologies studied and applied for the production of n-butanol.

The processing steps are discussed in more detail in the following paragraphs.

4.1.4.1. Feedstock Handling and Conditioning

In the mill process, after grinding the sugar cane, the bagasse left is carried through a series of conveyors directly to the boiler feeders or to a stockyard located close to the plant. For the production of n-butanol it is needed a system which deviates part of the bagasse to a concurrent conveyor, leading to the pretreatment plant (instead of the boilers). As the bagasse is already washed and chopped by the milling process, no further processing of the bagasse is needed prior to the feeding in the pretreatment reactor. The bagasse is brought by the conveyors, measured by inline scales, and an electromagnet is positioned to retain any metal parts that might have been carried by the conveyors and then bagasse is thrown into the screw conveyors to the pretreatment system.

4.1.4.2. Pretreatment

The objective of pretreatment is to separate the fraction of biomass called hemicellulose, which is the “softer” portion of biomass structure, being the easiest fraction to remove. For n-butanol production it is interesting to carry out this stage in the mildest conditions possible in order to avoid degradation of the hemicelluloses into chemicals such as furfural. The main reason is that the sugar yielded by hemicellulose, the xylose, is fermentable to n-butanol by some strains of bacteria, also, chemicals generated such as furfural have a potential to be inhibitant to the fermenting organisms.

Figure 4.2 shows a simplified flowsheet for the pretreatment, hydrolysis and separation of liquor.

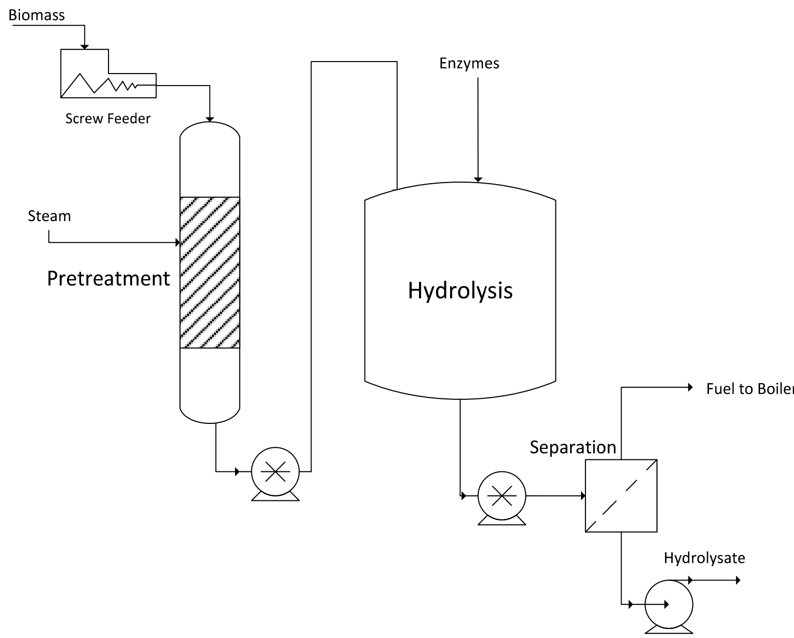


Figure 4.2 A Pretreatment and Hydrolysis sketch

Biomass is carried by conveyors to the screw feeders of the pretreatment system, these screw feeders guarantee the steady feeding of biomass and also the maintenance of the reactor's internal pressure by compressing the biomass during the feed. Pretreatment is carried out in a vertical continuous reactor, biomass is fed at the top of the column, descending as the reaction advances, steam is also injected at the top of the reactor.

The pretreatment technology chosen for this project is the hydrothermal pretreatment. In this technology, biomass is heated with water to temperatures that can range from 130 to over 200°C, the breakdown of biomass by heat generates acetic acid, which catalyzes further degradation of biomass, creating a feedback system. In this project, the pretreatment temperature is of 190°C (Bereche, 2011).

In the bottom of the reactor, a sludge is removed which contains solid lignin and cellulose and a hydrolysate juice containing hemicellulose polymers, xylose, some glucose and part of the lignin, this sludge is pumped to the hydrolysis reactor. Some energy recovery is obtained by flashing part of the water contained in the reaction. Depressurization is done from 4bar, which is the reaction pressure, to 1.2bar, a pressure that makes it possible for the use of this vapor in the process, this vapor is mainly used in the stripping of solvents after fermentation.

4.1.4.3. Hydrolysis

The objective of carrying out a hydrolysis process after pretreatment is to break down the cellulose into the glucose monomers and also finish the breakdown of hemicellulose into its monomers (xylose). Hydrolysis is carried out at mild temperatures, high residence times and in the presence of enzymes in CSTR type reactors. Since these reactors are usually very big due to the high residence times, this is an important step of the process cost wise.

After hydrolysis, a mechanical separation process is necessary to separate the hydrolysate juice containing the sugars desired and the residual solids, which are valued as fuel to complement the energy balance of the biorefinery. In this project, solid-liquid separation is considered to be carried out by filtration.

4.1.4.4. Hydrolysate Treatment and Conditioning

After hydrolysis, the hydrolysate juice obtained is not yet ready for the fermentation steps. In second generation ethanol production, simultaneous saccharification and fermentation process is considered as a method to integrate the two processes, improve kinetics since inhibitors are removed as they are consumed by the next process step. For the n-butanol production, the use of this method encounters technical barriers, since the butanol fermentation done by *clostridia* is more vulnerable to inhibitors and contamination than ethanol fermentation done by *Saccharomyces* yeast.

The higher vulnerability of the butanol fermentation brings up the need for conditioning the hydrolysate from biomass prior to the fermentation. This conditioning may include the removing of inhibitors, juice sterilization, and addition of nutrients, which in this example includes an addition of 10% of molasses over the sugar feed to the fermentation. In this project a sterilization step and mixing of the hydrolysate with molasses and nutrients is considered.

The hydrolysate is heated up to 130°C and held at this temperature for 30 minutes for sterilization purposes, heat recovery is performed and the hydrolysate goes to a mixing tank for the final tuning in nutrients and other additives such as antifoam. The Figure 4.3 shows the conditioning flowsheet configuration considered in this project.

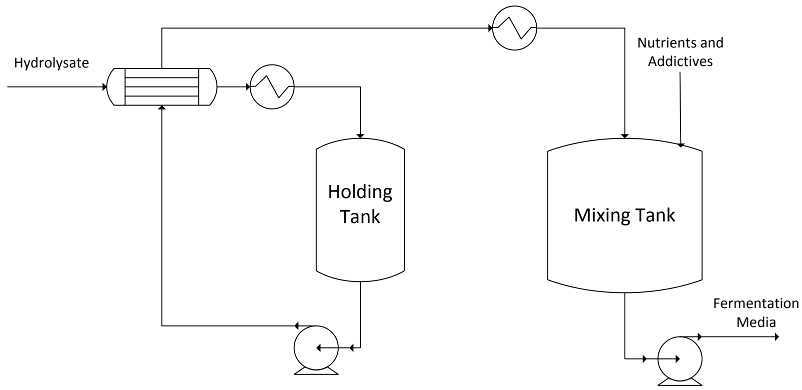


Figure 4.3 Hydrolysate Treatment and Conditioning Sketch

4.1.4.5. Fermentation

The conversion of sugars into butanol is done through a process known as ABE fermentation, in this work, fermentation process is considered to be similar to the processes known since the beginning of the XX century in spite of the different feedstock used.

The conditioned hydrolysate is fed to both the seed fermenters and the production fermenters. Seed fermenters are smaller than production fermenters and their purpose is to generate cells in a quantity sufficient to start the production fermenter at the optimum concentration of cells, conditions in the seed fermenters are the same as the production fermenters. Seed fermenters have also a safety purpose, i.e. if something goes wrong during cell growth, a smaller volume of media will need to be discarded.

Both the conditioned hydrolysate and the seed are then fed into the production fermenter, where the actual production of butanol happens. The fermentation is carried out at mild conditions, around 34°C and atmospheric pressure, residence time is around 24h of production fermentation (Mansur, et al., 2010).

Figure 4.4 shows a sketch for the ABE fermentation. The fermentation media is fed to both the seed fermenters and the production fermenters. The gases generated in the fermentation, mainly hydrogen and carbon dioxide, are then washed in a scrubber with water for solvent recovery.

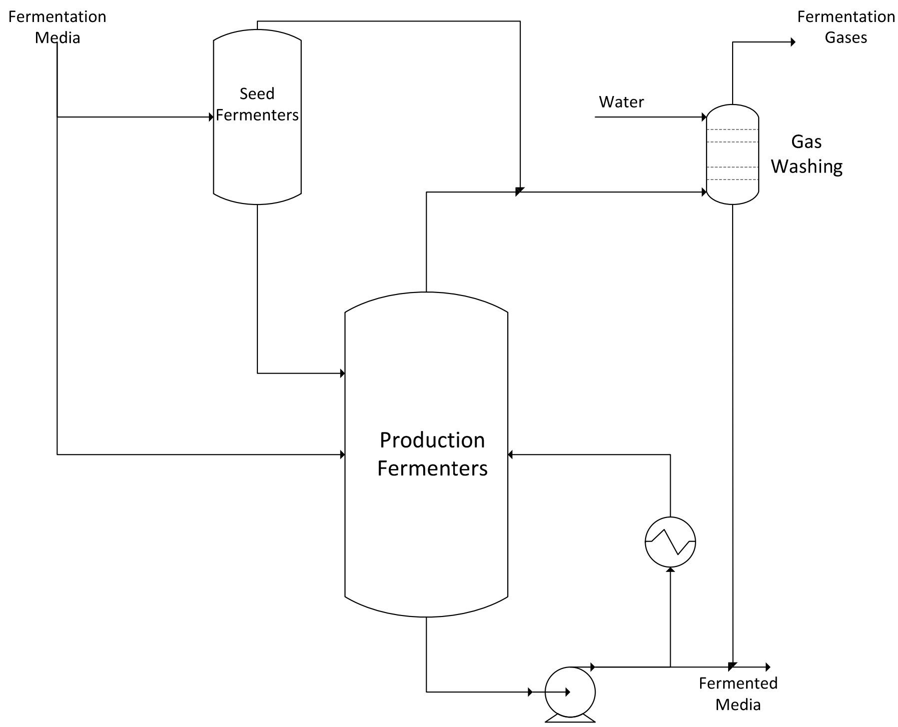


Figure 4.4 Sketch for the Biobutanol Fermentation with Seed

4.1.4.6. Separation

In this work, separation of n-butanol, acetone and ethanol is considered in this project to be done through a traditional distillation set, Figure 4.5 shows the distillation flowsheet.

Beer coming from the fermentation section goes through a couple of heat exchangers that heat up the broth using energy from both the condensers and vinasses, and then is fed to the first column (stripping) in which the solvents are stripped from water, n-butanol, acetone, ethanol and water are the light products. Vinasses is the bottom product, it is comprised mostly of the water from the broth, salts, heavy components generated by the cells, the cells itself, residual sugars and other organic matter carried from the biomass.

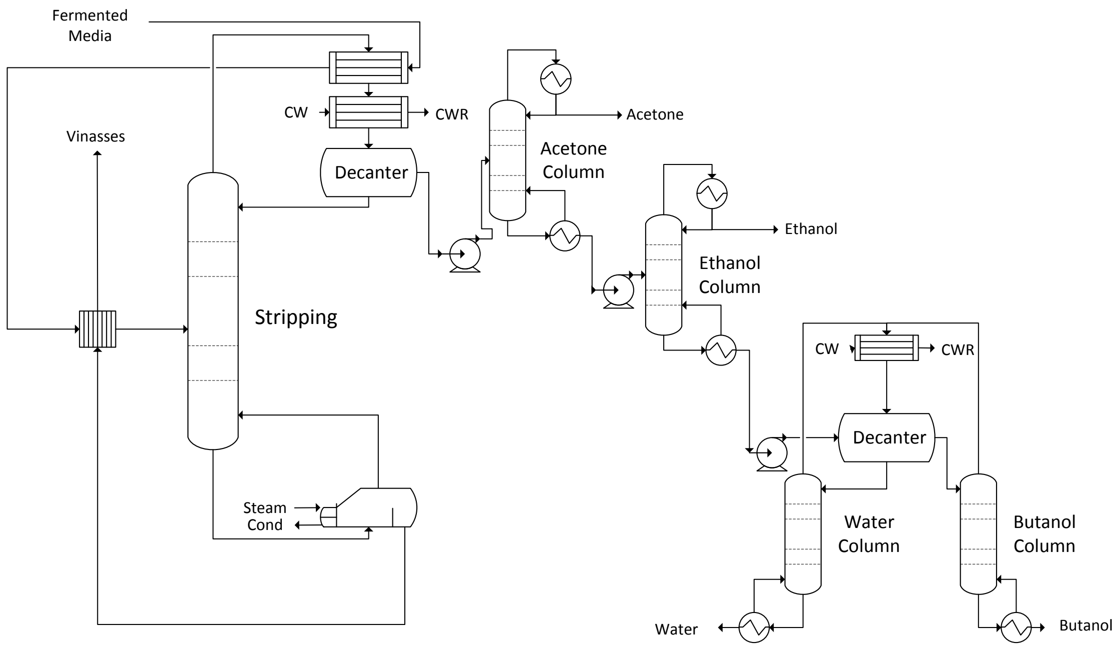


Figure 4.5 Sketch ofr the Solvent Separation Distillery

4.1.4.7. Utilities

The utilities section is composed mainly of the vinasses treatment system, due to the big dilution that is characteristic of fermentation processes, the ABE plant is both intensive in water need and generates a great amount of vinasses. The vinasses treatment system considered is a multiple effect evaporator as shown in Figure 4.6.

Evaporating the water from the vinasses has some benefits, one of them being the reuse of the condensate as process water and reduction of the vinasses volume for dispersion or disposal. But other processes can be considered in this case such as membrane filtration, bio digestion, etc.

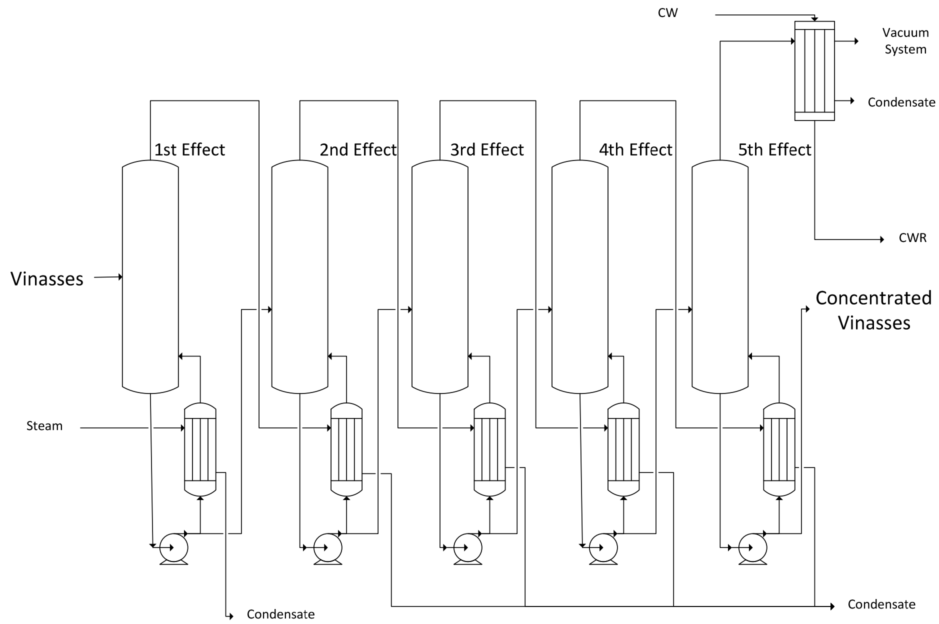


Figure 4.6 Vinasses Concentration System

4.2. Base case application and analysis;

In order to analyze the integration of a biobutanol producing plant using a sugarcane mill as a biorefinery, lignocellulosic sugars as feedstock and ABE technology, mass and energy balances of both the mill and the biobutanol plant were buit as described in Chapter 3. Two production scenarios should be analyzed taking into account the market demanded amount of butanol and also, the maximum biobutanol production achievable with a regular sugarcane mill existing in Brazil, these being the most probable partner for a biorefinery installation. The market size for biobutanol is around 80kt/y after market information from such projects emerging in Brazil (ICIS, 2011) and the scenario respective to a biobutanol plant achieving this production volume is named Scenario 1. A sugarcane mill of average crushing capacity of 3.5 million tons/y of sugarcane is considered in Scenario 2, and the biobutanol production to match such sugarcane mill is defined at 30.1kt/y, meaning that two different scales of the biorefinery were evaluated.

Figure 4.7 shows the decision flowchart in the analysis of the biorefinery, both the economics for the mill in its original configuration and for the biorefinery are calculated and compared to determine if the addition of the biobutanol plant improves or deteriorates the results. The risk analysis (named 1st Simulation Run) is run afterwards, the probabilities of achieving the intended economic results are evaluated and the most influential variables relative to the targeted results are observed. Critical analysis of such variables should determine which ones should be redefined in order to refine the analysis, a second risk analysis (named 2nd Simulation Run) is done with the refined variables and its results evaluated.

The objective of the whole exercise is to determine the probability of success of the project and to which aspects of it one should dedicate stronger efforts. For example, if process parameters such as efficiencies and consumptions are found to be very influential, research efforts should be directed into investigating such parameters, if economic inputs such as prices of raw material or products are found to be most influential, market efforts to better understand such prices should be employed.

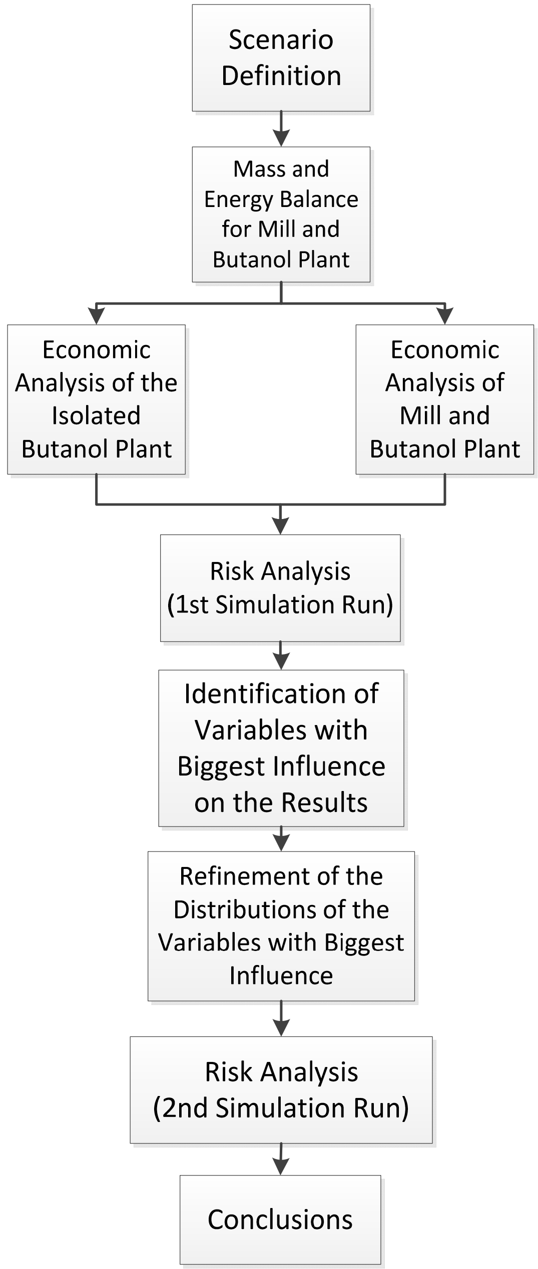


Figure 4.7 Method for the Feasibility Analysis of a Biobutanol Plant

In Figure 4.7, it is shown that two economic analyses are done in parallel: of the biobutanol plant as an isolated venture and the transformation of the sugarcane mill into a biorefinery, or a mill plus biobutanol plant venture. When analyzed from the perspective of the whole biorefinery, there are specificities to the economic analysis; the transformation of a regular sugarcane mill into a biorefinery means that less electricity will be exported by the mill and in the same amount it will be transferred to the biobutanol plant via heat and electricity. It is also expected a small reduction of ethanol output from the mill after integration, since a small part of molasses is diverted to the biobutanol fermentation in order to aid with its salts and nutrients balance.

4.2.1. Premises and Inputs;

As described in section 2.4.3, when assigning distributions to the variables of the model for risk analysis, the analyst should evaluate first if information is available in order to determine the distribution. If historical data is available, it is possible to determine the distribution that best fits the data, and such distribution can be used in the risk analysis, in early stage project analysis, historical data might be available only for the variables involving prices. For technical data, the guidance explained in the section 2.4.3 should be used, since there shouldn´t be any lab or pilot data available for the analyst in the very beginning of a project.

4.2.1.1. Butanol Price;

Butanol is a well-known chemical, meaning that it is possible to obtain the historical data for its price. In this example, data for butanol prices were retrieved for the last 10 years in the AliceWeb database (AliceWeb, 2015), this database gathers information of volume and prices of goods being imported and exported in Brazil. Figure 4.8 shows a histogram of the butanol prices for this time period.

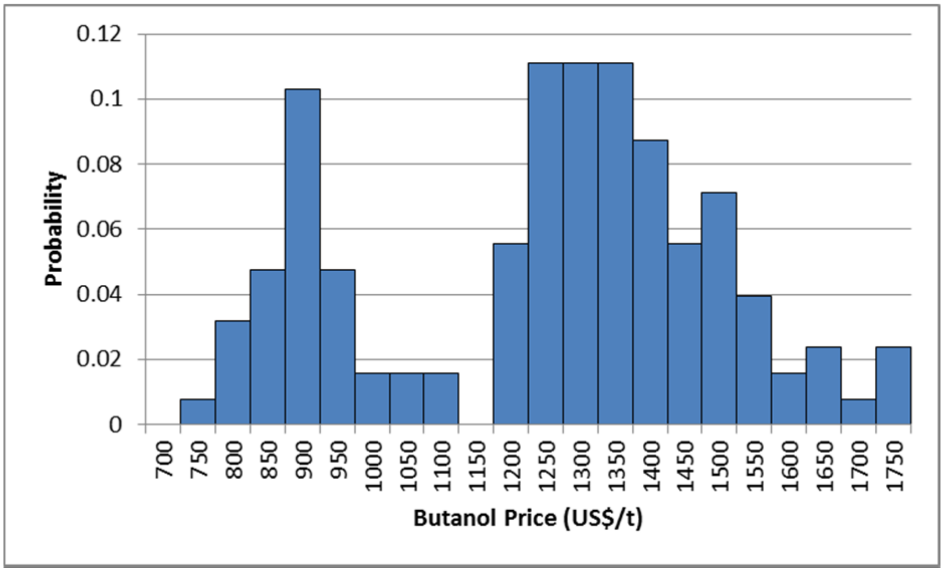


Figure 4.8 Butanol Price (US$/t) Distribution in Ten Years Spam (2005-2015). (AliceWeb, 2015)

In order to facilitate the insertion of the butanol price distribution in the risk analysis, the software @Risk was used to identify the best distribution model fit for the historical data retrieved. The software @Risk uses the AIC (Akaike Information Criterion) methodology to select the model that best fits the data. In the case of butanol price data, it´s possible to see that a single distribution will not fit the data well, since there are two distinct groups of values. The alternative chosen was to make two distribution fits, one for the lowest butanol prices and another for the highest; the final butanol price used in the risk analysis was done by shifting between the two distributions by using a random number generator. In this set of data, 28% of the values belonged to the lower set, under US$1150/t, and 62% belongs to the higher group above US$1150/t, if the random number resulted lower than 0.28, the lower set was chosen, if higher, the higher set was chosen. The result of this attempt to best reproduce the butanol price in Brazil is shown in Figure 4.9.

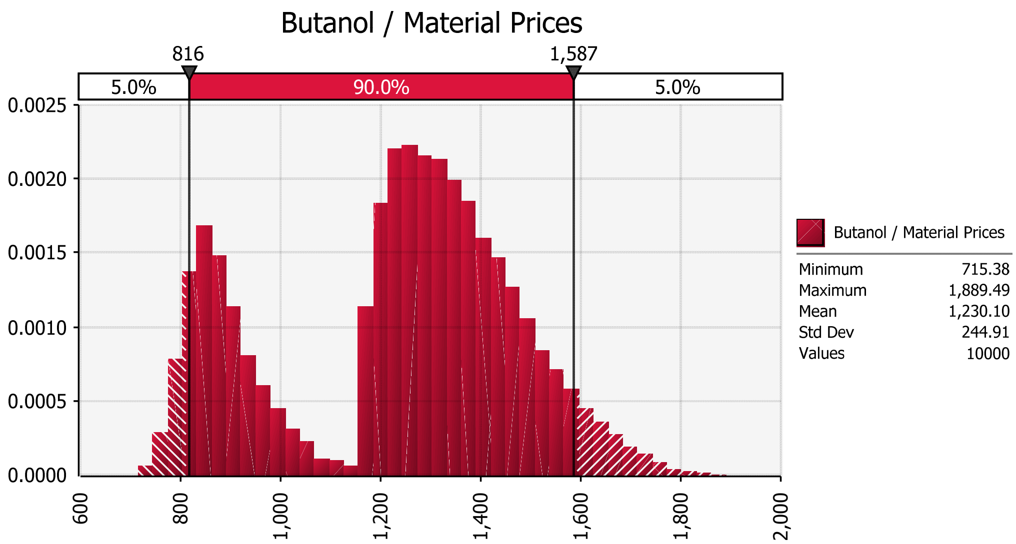


Figure 4.9 Distribution for Butanol Price (US$/t) after Division into a Lower and a Higher set of Prices.

4.2.1.2. Acetone Price;

The same process of price distribution definition was applied for acetone, data for acetone price in Brazil for the last 10 years was retrieved in the AliceWeb system (AliceWeb, 2015).

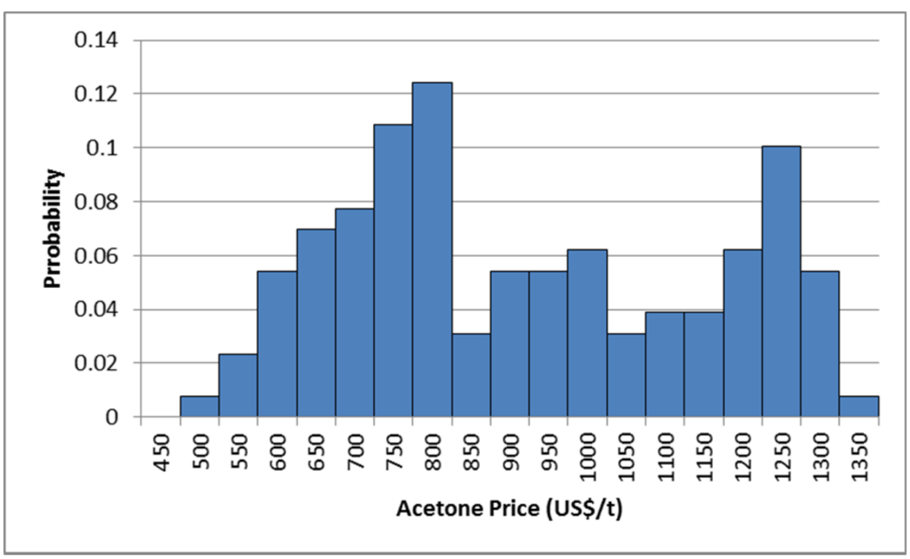


Figure 4.10 Acetone Price (US$/t) Distribution in Ten Years Spam (2005-2015) (AliceWeb, 2015)

Similarly to the butanol price distribution, it was possible to identify two peaks of sets of data in the acetone data, indicating that dividing the data into two tiers is probably a better approach. The data was divided in lower than US$1050/t and higher, being 70% of the data below US$1050/t and 30% higher, the same random number generator used in the butanol distribution was used to choose between the two sets of acetone price data. The result of this exercise is shown in Figure 4.11.

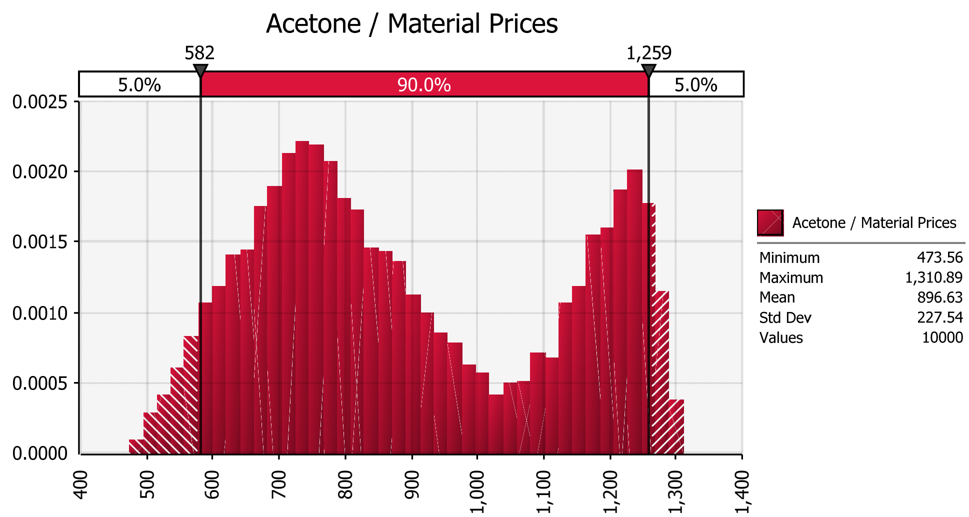


Figure 4.11 Distribution for Acetone Price (US$/t) after Division into a Lower and a Higher Set of Prices

4.2.1.3. Ethanol Price;

Ethanol price data was obtained for the last 12 years was obtained in the CEPEA (Center for Advanced Studies in Applied Economy). The center integrates the University of São Paulo school of Agriculture Sciences (ESALQ) and monitors the prices of the various grades of ethanol and sugar produced by the sugarcane mills. The data on ethanol price was used to obtain the distribution in the same fashion as with butanol and acetone prices only without the need of dividing the data into two sets, a fit was found for the whole set of data.

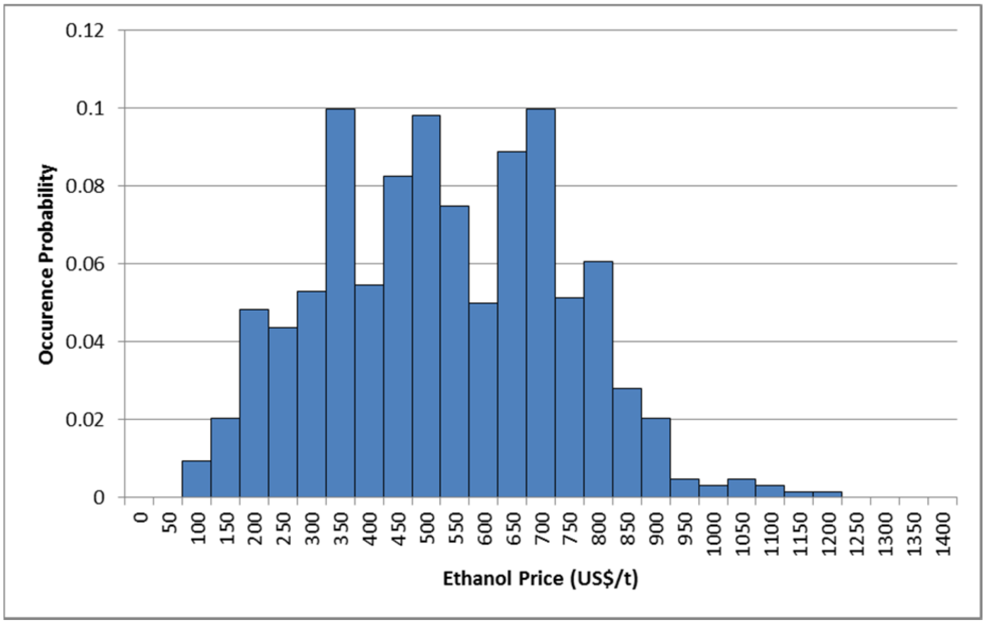


Figure 4.12 Ethanol Price (US$/t) Distribution for a Twelve Year Spam (2003-2015) (CEPEA, 2015)

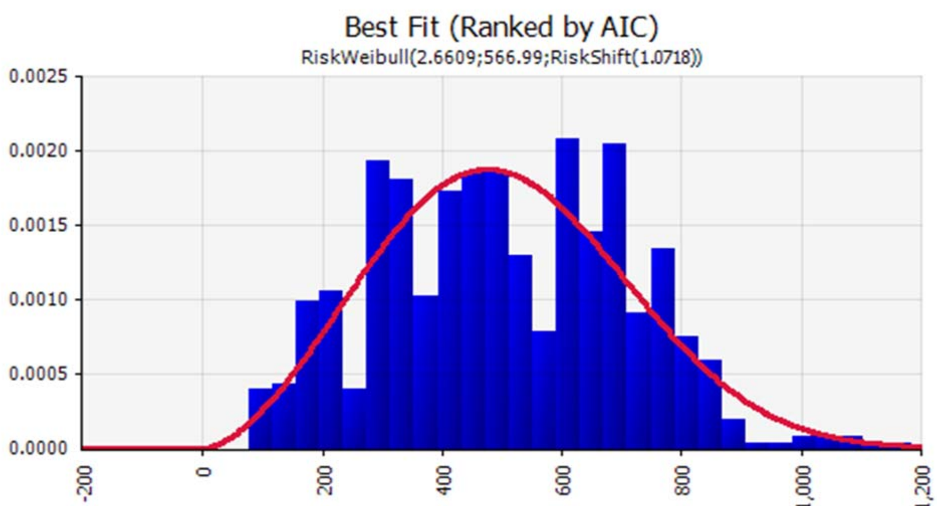


Figure 4.13 Distribution Fit Adjusted for Ethanol Price (US$/t) using @Risk

The distribution best found to fit the historical data for ethanol price is the Weibull and the most probable value lies around US$500/t, as shown in Figure 4.12 and Figure 4.13.

4.2.1.4. Sugar Price;

Sugar price data for the last twelve years was also retrieved from the CEPEA site, and its distribution fit obtained from the @Risk software with AIC methodology.

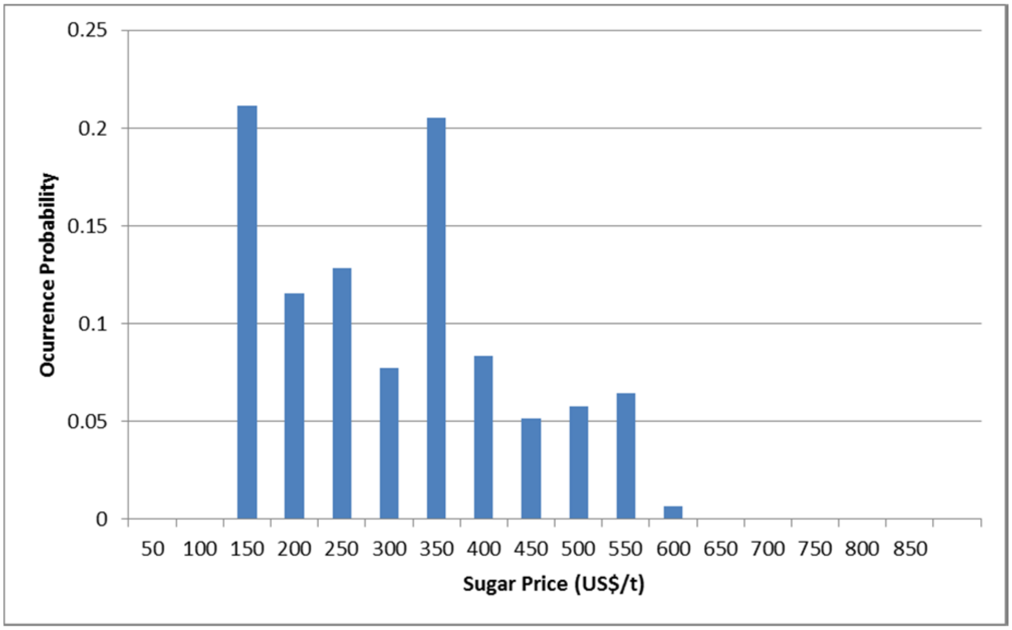


Figure 4.14 Sugar Price (US$/t) Distribution in a Twelve Year Spam (2003 – 2015) (CEPEA, 2015)

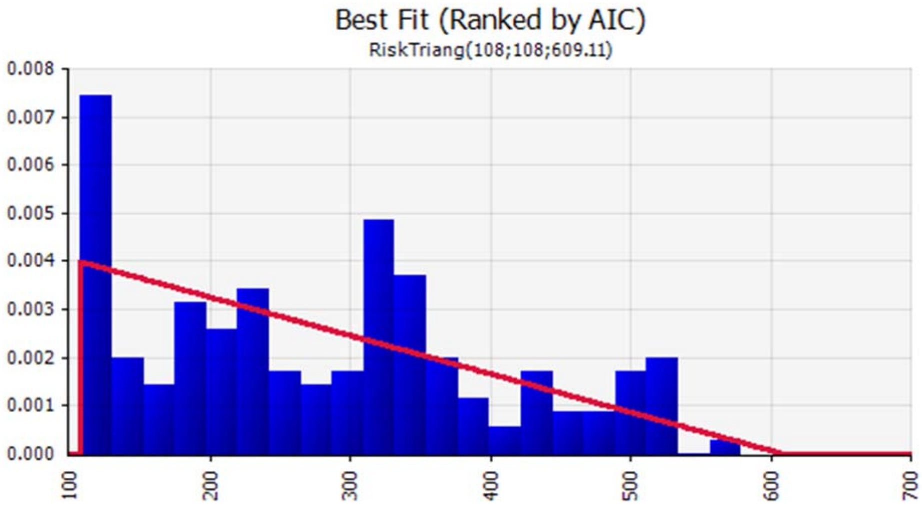


Figure 4.15 Distribution Fit for Sugar Price (US$/t) Obtained with @Risk

The distribution fit obtained is a triangular one, with the highest probability of occurrence near the US$100/t as shown in Figure 4.14 and Figure 4.15.

4.2.1.5. Enzyme Price Discussion;

To identify the distribution for enzyme price is not as straightforward as it is for products such as butanol, acetone and ethanol. From the literature it is possible to infer a high variability of values.

Klein-Marcushamer et al (2011), in the study *The Challenge of Enzyme Cost in the Production of Lignocellulosic Biofuels* argues that many authors don´t even consider enzyme price to be an important factor in the economic analysis of such projects due to belief that technological advancements will lower enzyme price significantly and in many cases the use of enzyme cost values in US$/gal of ethanol makes the exercise of defining enzyme cost confusing. A low price based on soy protein cost and a high price based on simulation of enzyme production from steam exploded wood are calculated, the low value obtained is US$1.25/kg and the high value US$10.14/kg.

Albarelli, (2013) in the thesis *Produção de Etanol de Primeira e Segunda Geração: Simulação, Integração Energética e Análise Econômica* also tackled the issue of enzyme prices, making a sensitivity analysis considering the highest enzyme price US$10.14/kg, from the work by Klein-Marcushamer and a lowest enzyme price of US$0.12/kg, used by other authors to evaluate second generation ethanol processes. The economic analysis showed the importance of the enzyme price on the feasibility of second generation ethanol, especially because of the big discrepancy between the lower and the higher values.

Considering the information obtained from these two works, for the first risk assessment, it was considered a triangular distribution with the highest probability around US$10.14/kg and the lowest probability around US$0.12/kg, the high value obtained by simulation of the actual enzyme production process, thus being considered the most accurate evaluation of the enzyme price.

Figure 4.16 shows the distribution of enzyme price considered in the first assessment.

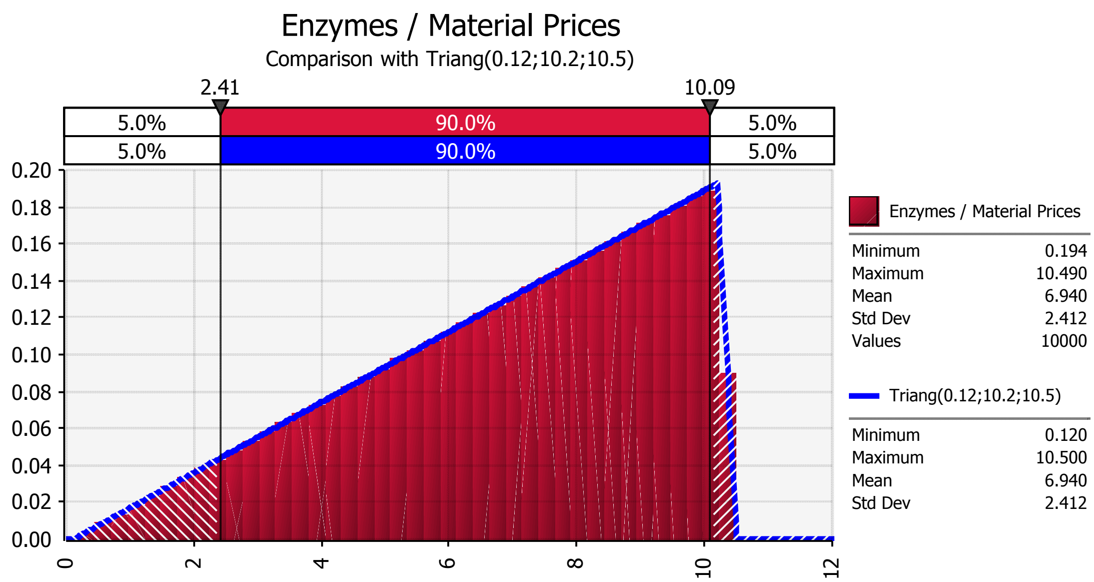


Figure 4.16 Enzyme Price (US$/kg) Distribution and Fit obtained with @Risk

4.2.1.6. Utilities Price Discussion;

One of the objectives of this work is to analyze the biobutanol plant individually, and to do this it is necessary to estimate electricity and steam prices even though they are generated inside the mill into which the biobutanol plant will be annexed.

Electricity price was estimated to be around US$65/MWh based on values obtained in recent selling auctions for biomass electricity projects, and steam price was estimated by opportunity cost. Since steam is used to generate electricity in the mills, steam price was estimated considering how much could be gained by each ton of steam if it was to be used to generate electricity. To produce one megawatt-hour, it is needed approximately four tons of steam, so the price to be paid for one ton of steam was estimated to be one quarter of the price of one megawatt-hour, coming to a value of US$16.5/t of steam.

To make an accurate estimation of steam and electricity costs for the biobutanol plant, it would take a comprehensive economic analysis of a combined heat and power plant, taking into account fixed costs and depreciation of equipment. For an early stage analysis, one should avoid employing such amount of effort to obtain distributions for such variables in the first analysis. Such an effort should be done in a second round of analysis only if these variables prove to be influential in the economic results of the biorefinery.

Since values for electricity and steam are estimated, a normal distribution was assigned for both; the distributions are shown in Figure 4.17 and Figure 4.18.

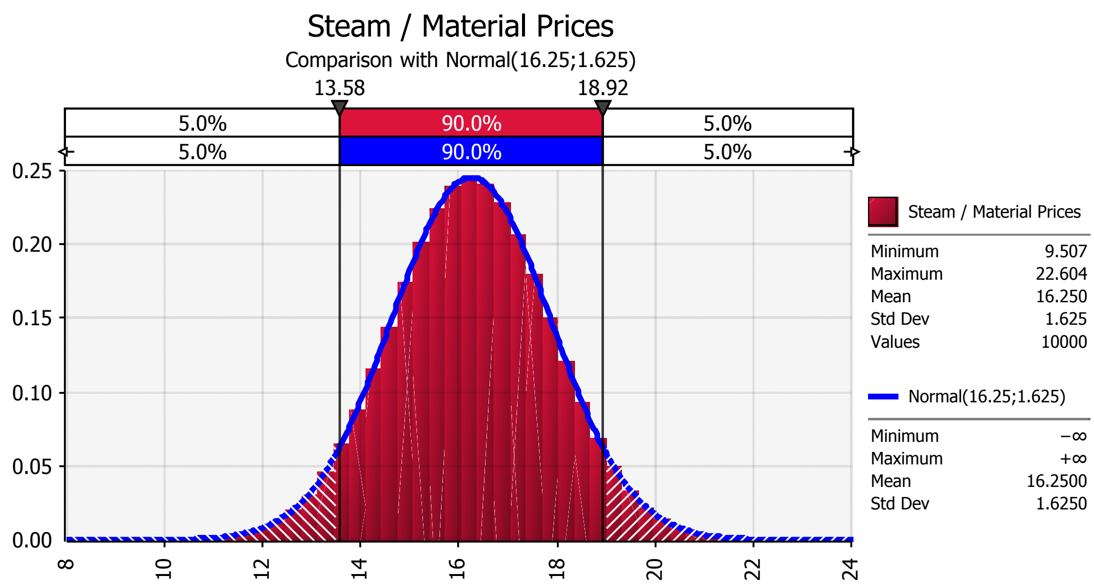


Figure 4.17 Steam Price (US$/t) Distribution

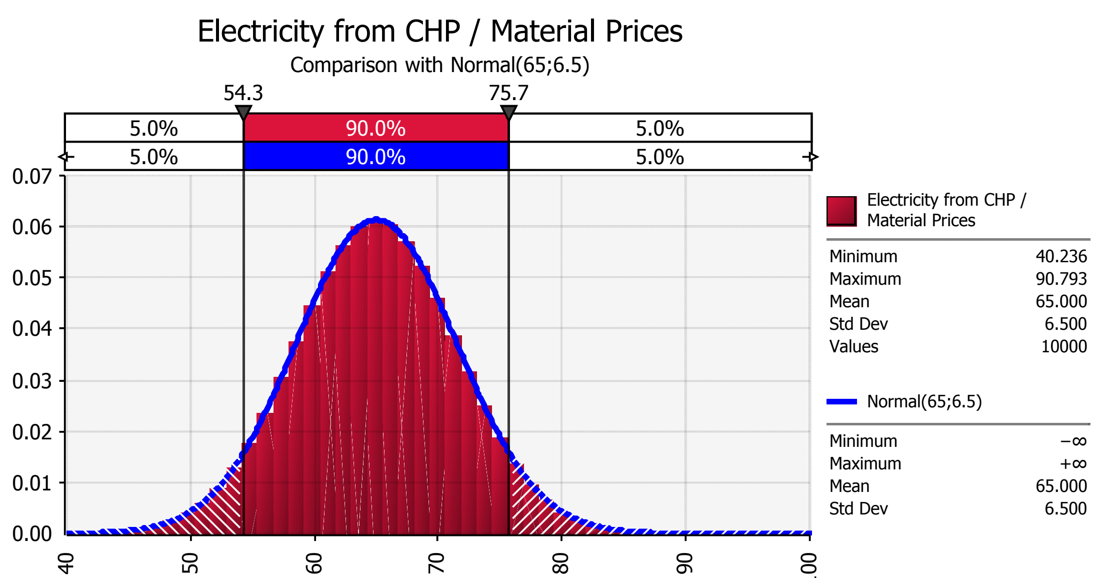


Figure 4.18 Electricity Price (US$/MWh) Distribution

4.2.1.7. Biomass Price Discussion;

A range of values can be found in literature for biomass cost to the plant ranging from US$15/t to US$60/t (dry basis) (Mariano, et al., 2013) (Gnansounou, et al., 2010) (Dias, et al., 2011) (Treasure, et al., 2014). The value used in the first analysis is US$25/t (dry basis) and a normal distribution was assigned to this variable. In the same way as electricity and steam prices, biomass costs to the plant can also be estimated through comprehensive analysis of plantation and logistics costs, but such an effort should not be employed in early stage analysis unless it is proven to be a variable of strong influence in the economic feasibility of the project. Figure 4.19 shows the distribution for the biomass price.

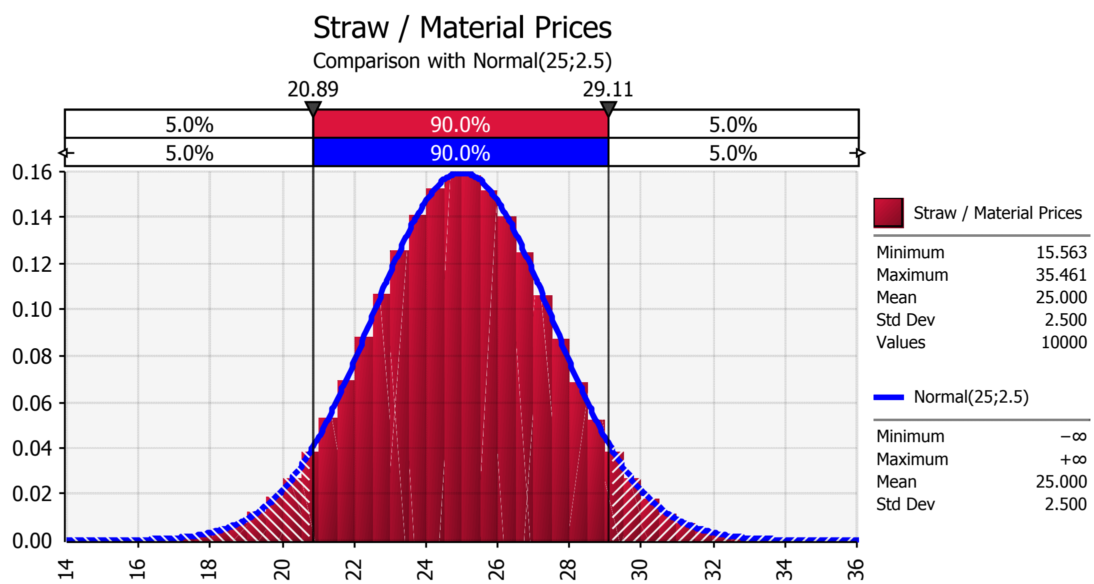


Figure 4.19 Biomass Price (US$/t) Distribution

4.2.1.8. Process Parameters;

As explained in section 2.4.3, most variables in the analysis in early stages are estimated using experience, literature or databanks, since there won´t probably be experimental data to rely on at this point. For the risk analysis, a distribution must be assigned to each variable, so in the absence of historic or experimental data, normal or triangular distributions could be assigned according to the experience of the analyst. Table 4.1 summarizes the distributions assigned to parameters concerning the mass and energy balance and the economic analysis of the biobutanol plant.

Table 4.1 Summary of the Input Distributions for Process and Project Parameters

Name	Distr	Min	Mean	Max
Bagasse in Mix (%)	Uniform	0.0	50	99
Cellulose Conversion (%)	Normal	32.8	55.8	78.2
Hemicellulose Conversion (%)	Normal	24.8	40.6	57.3
Steam Consumption (t/tsolids)	Normal	0.33	0.55	0.76
Concentration (% solids)	Discrete	5	10	15
Enzyme Cons (% over Cellulose)	Triangular	4.0	11.4	11.5
Fermentation Efficiency (%)	Normal	62.4	78.0	93.2
Butanol Ferm Concentration (%)	Normal	0.93	1.5	2.1
Fermentation Time (h)	Normal	18.3	29.9	41.5
Development Fees (%)	Discrete	2.4	5.2	10.0
Reserarch Costs (kUS$)	Normal	746.7	1300.0	1800.0
Research Time (y)	Discrete	2	3	4
Industrialization Time (y)	Discrete	2	3	4
Years from First Sales to Max (y)	Discrete	2	3	4
Capex Innacuracy Factor	Triangular	0.6	1.05	1.5

4.2.2. Mass and Energy Balance Results;

The most important premise adopted in defining the scenarios for mass and energy balance is that the butanol plant should be added to a mill large enough to eliminate the need to buy biomass from crops outside those that already provide sugar cane to the mill.

According to media reports, butanol demand in South America is around 80kt/y (ICIS, 2011), the first scenario considers this production for the biobutanol plant, and a mill with a crushing capacity of over nine million tons of sugarcane per year was calculated as necessary to accommodate such plant.

Nine million tons of cane per year is arguably a mill too big for Brazillian standards, so a second scenario was defined in order to represent what would be an integrating option for an average Brazilian sugarcane mill. An annual crushing capacity of three and a half million tons of sugarcane per year was considered in scenario two, and thus the biobutanol plant capacity was sized accordingly. The add-on biobutanol plant for this scenario has a production capacity of 30.1kt/y.

A annual crushing season of 220 days was considered with a 90% availability of the mill, resulting in operating hours of 4750 h/y.

The main numbers for scenarios one and two are shown in Table 4.2.

Table 4.2 Mass and Energy Balance Results for the two Scenarios

	Scenario A		Scenario B	
Data	Mill	Mill + Biobutanol	Mill	Mill+Biobutanol
Biobutanol Production (kt/y)	-	80.0	-	30.1
Acetone Production (kt/y	-	40.4	-	15.2
Mill Crushing Capacity (Mt/y)	9.06	9.06	3.5	3.5
Sugar Production (kt/y)	844.3	844.3	326.1	326.1
Ethanol Production (kt/y)	214.8	211.5	82.9	81.2
Steam Generation (t/h)	1463	1124	565	438
Power Generation (MW)	298.4	178.7	115.3	69.5
Power Consumption (MW)	39.8	64.2	15.4	24.9
Power Export (MW)	258.6	114.5	99.9	45.1
Biomass to Butanol Plant (Dry t/h)	-	176.0	-	66.2

The numbers displayed in Table 4.2 shows the main impacts on the mill mass and energy balance when the biobutanol plant is added. The main impact clearly is the reduction of biomass available for energy generation, since biomass will be used for production of chemicals. Results in Table 4.2 consider that the mill already used straw to produce electricity, and straw availability is half of bagasse availability in terms of dry biomass. If the premise taken is that the mill used only bagasse to produce electricity, then biomass use for chemicals can be compensated by straw.

Table 4.3 shows the specific consumptions of the biobutanol plant.

Table 4.3 Biobutanol Plant Specific Consumptions

Data	Consumption
Biomass (t/t of Butanol)	10.5
Enzyme (t/t of Butanol)	0.1
Water (t/t of Butanol)	14.4
Electricity (MWh/t of Butanol)	1.6
Steam (t/t of Butanol)	23.0
Effluent Treatment (t/t of Butanol)	5.3
Solids to Fuel (t/t of Butanol)	5.5

The biomass feed to the plant needed is 10.5 mass units of biomass by mass unit of butanol, after pretreatment and hydrolysis 5.5 mass units residual solids per unit of butanol are sent back to the boiler, meaning that 5 mass units of biomass is consumed to produce one mass unit of butanol.

Steam consumption is a very important factor in the mass and energy balance and integration with the mill because it determines, together with the biomass intake into the biobutanol plant, the necessary crushing capacity of the mill so that external biomass is not necessary to run the process.

Table 4.4 shows the steam consumption of the biobutanol plant divided in the three main consuming areas: pretreatment/hydrolysis, media treatment and distillation.

Table 4.4 Specific Steam Consumptions of the Biobutanol Plant

Area	Consumption
Pret/Hydrolysis (t/t of Butanol)	8.3
Distillation (t/t of Butanol)	10.5
Media Treatment (t/t of Butanol)	4.2

Pretreatment and hydrolysis steam consumption were determined in the work of Bereche (2011) as all data concerning mass and energy balance for this process.

Media treatment and distillation steam consumptions were determined by energy balances.

4.2.3. Economic and Risk Analysis;

Economic and risk analysis were performed for the two scenarios described in section 4.2.2 to calculate the probability of economic feasibility being achieved for an add-on process to a biorefinery.

In order to study the integration of the new process to an existing mill, economic results for both the biobutanol plant isolated, represented by the “biobutanol plant” box in Figure 4.1 and the whole biorefinery, represented by the sum of the boxes “mill” and “biobutanol plant” in Figure 4.1 will be analyzed. The objective is to determine if the synergy between mill and biobutanol plant would result in better chances of feasibility in a project where the mill and biobutanol plant are owned by the same investor than when the investor owns the only the biobutanol plant. In the analysis, for every result that is presented to the biobutanol plant, another will also be presented representing the project of integrating the biobutanol plant into the mill.

The integration project takes into account that an investment will be made to build a biobutanol plant inside the sugarcane mill. The financial gain of the project will be the extra income from butanol; reduction of income relative to the reduction of electricity sold to the grid and reduction of ethanol production because of the use of molasses for media composition in the ABE fermentation is also accounted for. The operational costs of the integration project are the delta of variable costs and fixed costs brought by the installation of the biobutanol plant.

The biobutanol plant will be first analyzed as an independent venture, buying raw material and utilities to produce solvents, then economic figures for the whole of the biorefinery are calculated and compared to the original economic indexes of the mill, in this work this numbers a referred to as integration indexes. It should be possible to observe with these integration results what costs are aggregated to the biorefinery by the add-on plant, what are the incomes added and if the balance of added costs, incomes and investment yield a feasible scenario for the biorefinery owner.

4.2.3.1. Scenario A

In the Scenario A, a biobutanol plant with production capacity for 80kt/y is integrated with a sugarcane mill with crushing capacity for 9.06Mt/y of sugarcane. Investment was estimated for the inside battery limits (ISBL) of the plant, meaning the process steps for transforming biomass into solvents. Outside battery limits (OSBL), being the connections, facilities and utilities were considered to be 50% of the ISBL (Bray, 2007). The ISBL costs were estimated using the process step score (Taylor, 1977) as explained in section 2.3.1.2.

Variable costs were calculated according to the consumptions calculated by mass and energy balance and values discussed in sections 2.3.2 and 4.2.2. Fixed costs for the biobutanol plant were defined according to Table 4.5.

Table 4.5 Fixed Costs for the Biobutanol Plant for Scenario A

Fixed Cost Butanol Plant	
Shifts	4
Operators	9
Hours (h/year)	2288
Cost (US$/h/operator)	11.7
Total Operation Cost (US$/y)	963,706
Overheads (% of Operation Cost)	100%
Site Maintenance (US$/y)	500,000
Maintenance (% of ISBL)	2%
Total Fixed Costs (US$/y)	4,734,748

The costs of labor in Brazil were taken from a research by the Bureau of Labor Statistics (BLS), that presents labor cost data from many different countries up until 2013 (Bureau of Labor Statistics, 2013). In the same way, variable costs were calculated according to the mass and energy balance of the mill and fixed costs were determined according to Table 4.6, the same labor costs of the biobutanol plant were used.

Table 4.6 Fixed Costs for the Mill Prior to Integration for Scenario A

Mill Fixed Costs	
Shifts	4
Operators	26
Hours (h/year)	2288
Cost (US$/h/operator)	11.7
Total Operation Cost (US$/y)	2,784,038
Overheads (% of Operation Cost)	100%
Site Maintenance (US$/y)	1,000,000
Maintenance (% of ISBL)	2%
Total Fixed Costs (US$/y)	6,568,077

Table 4.7 summarizes the costs and income of the biobutanol plant, mill and integrated biorefinery. The costs for the biobutanol plant are calculated having the butanol production as basis, whereas the costs for the mill and the biorefinery have the sugar production as basis, making it possible to directly compare the costs and incomes for the mill and for the biorefinery after integration with the biobutanol plant.

Table 4.7 Costs and Income for the Biobutanol Plant, for the Mill Originally and for the Biorefinery (Mill + Biobutanol Plant) for Scenario A

	Biobutanol Plant	Mill	Biorefinery
Variable Costs (US$/t of Butanol)	1657		
Variable Costs (US$/t of Sugar)		346	443
Fixed Costs (US$/t of Butanol)	59		
Fixed Costs (US$/t of Sugar)		8	13
Depreciation (US$/t of Butanol)	216		
Depreciation (US$/t of Sugar)			20
Investment (MUS$)	173		173
Income (US$/t of Butanol)	1893		
Income (US$/t of Sugar)		535	646
Margin (US$/t of Butanol)	-40		
Margin (US$/t of Sugar)		181	169

It is possible to observe from Table 4.7 that the operating costs are increased when the biobutanol plant is integrated to the mill, and a depreciation cost is added to represent the loss of value of the assets of the biobutanol plant. The income of the plant also increases in the biorefinery, meaning that the loss of income with the reduction of electricity sold to the grid is compensated by the income with the butanol, acetone and ethanol produced in the ABE plant.

The economic results are shown in Table 4.8.

Table 4.8 Economic Results for Scenario A

	Biobutanol Plant	Integration
NPV (MUS$)	-111	-28
IRR (%)	-	-
EBITDA (MUS$)	0	23

The values presented as in Table 4.7 and Table 4.8 might give the project team the impression of a false precision. However, it is important to keep it clear that there is a great deal of imprecision in these numbers due to the fact that the project under evaluation is in its early stages of development and, therefore, all of the inputs and premises have an important amount of uncertainty. Also, given the economic results presented in Table 4.8 one might deem this project as not economically feasible, stopping any further work on it.

The risk analysis expresses the uncertainties of the project results by presenting not a value of the metric being observed but a distribution of such metric. By studying the distribution it is possible to the team working on a project can understand the results and probabilities that such project can achieve. Another output of the risk analysis is the identification of the main variables impacting in the economic results of the project; this information adds a greater depth to the analysis.

The Net Present Value (NPV) distribution obtained for the biobutanol plant is shown in Figure 4.20.

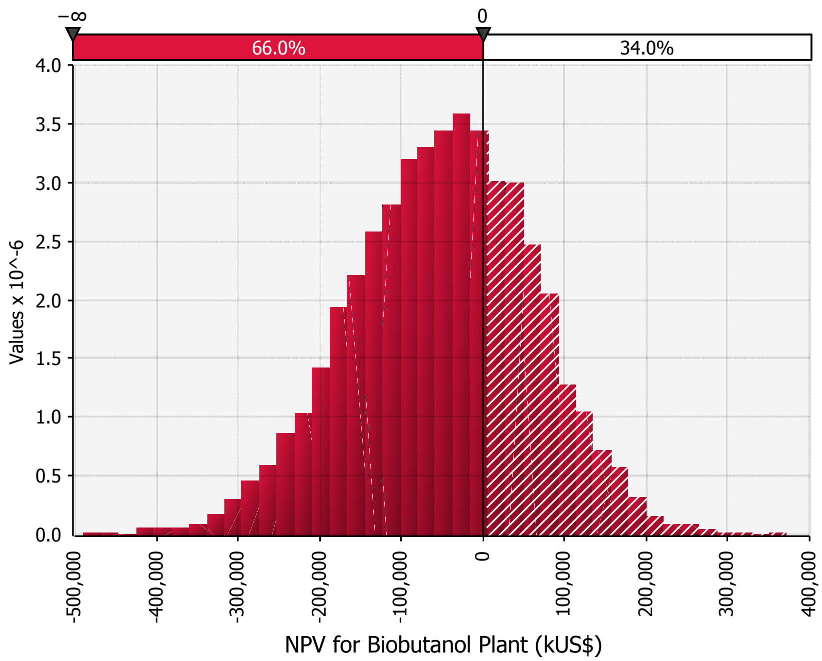


Figure 4.20 Net Present Value Distribution for a Biobutanol Plant Project for Scenario A

In Figure 4.20 it is possible to observe the distribution of Net Present Values (NPV) for the biobutanol plant. The distribution is fairly broad as inputs are also broad, as the projects advances and certainties on inputs grow; there is a tendency of the distribution to become less broad and more precise. Even though the distribution is large, it is already possible to infer important information from this result, the most important being that the probability of achieving a positive NPV is 34%. This graph was obtained through a Monte Carlo simulation running 10,000 calculations, meaning that the mass and energy balances and economic analysis was done 10,000 times with 10,000 different inputs obeying the distributions and probabilities determined by the user. A 34% probability of achieving a positive NPV means that of the 10,000 calculations done in the Monte Carlo run, only 3,400 yielded a positive NPV.

Figure 4.21 presents the NPV for the investment of a regular sugarcane mill into a biorefinery.

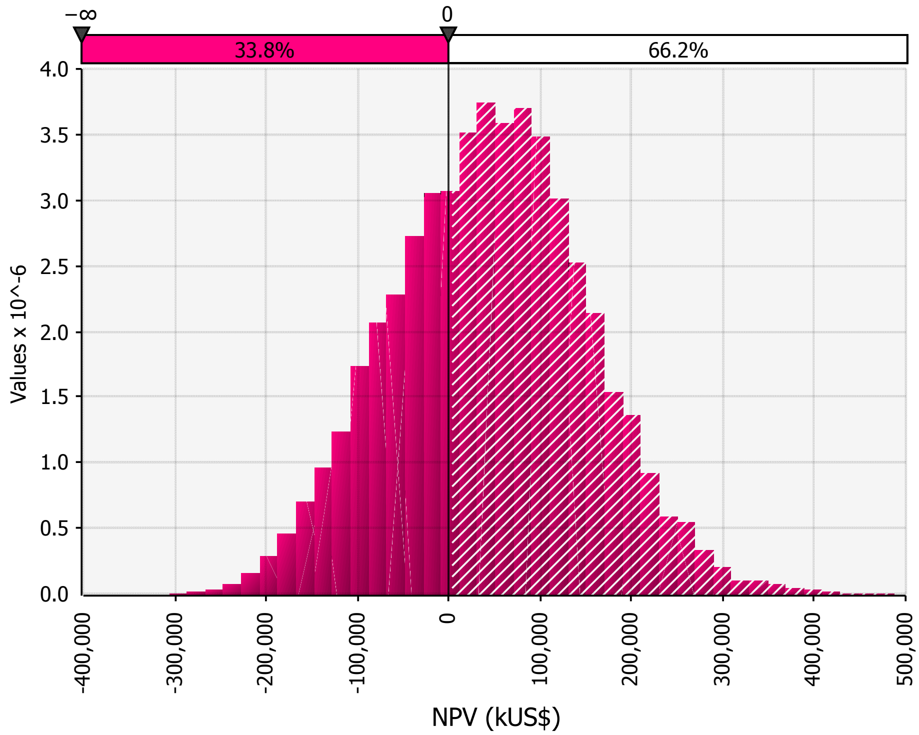


Figure 4.21 Net Present Value of the Investment in Integrating a Mill to a Biobutanol Plant for Scenario A

Figure 4.21 represents the same economic measurement as in Figure 4.20, but in this case the calculation of the Net Present Value accounts not only for the biobutanol plant but for the whole changes in the mill economic profile to become a biorefinery. The NPV distribution in Figure 4.21 points out to the conclusion that looking into the project as a complement to an existing mill yields better results than considering it as an isolated venture. This difference comes from the pricing power of the utilities that the mill sells to the biobutanol plant versus the price of electricity that the mill sells to the grid. In section 4.2.1.6 it was discussed how utilities such as steam are priced as opportunity, meaning that they are priced around the value that the mill could extract from such steam if it decided to generate electricity and sell it to the grid. As the Monte Carlo analysis was run, steam and electricity prices varied according to the distributions defined in the inputs, when steam prices were more economical than electricity, NPV of the mill plus biobutanol scenario became more attractive than the biobutanol plant isolated and when steam prices were less economical than electricity, NPV of the isolated biobutanol plant was higher than that of the mill plus biobutanol plan analysis. Figure 4.22 shows the overlapping of the two NPV distributions.

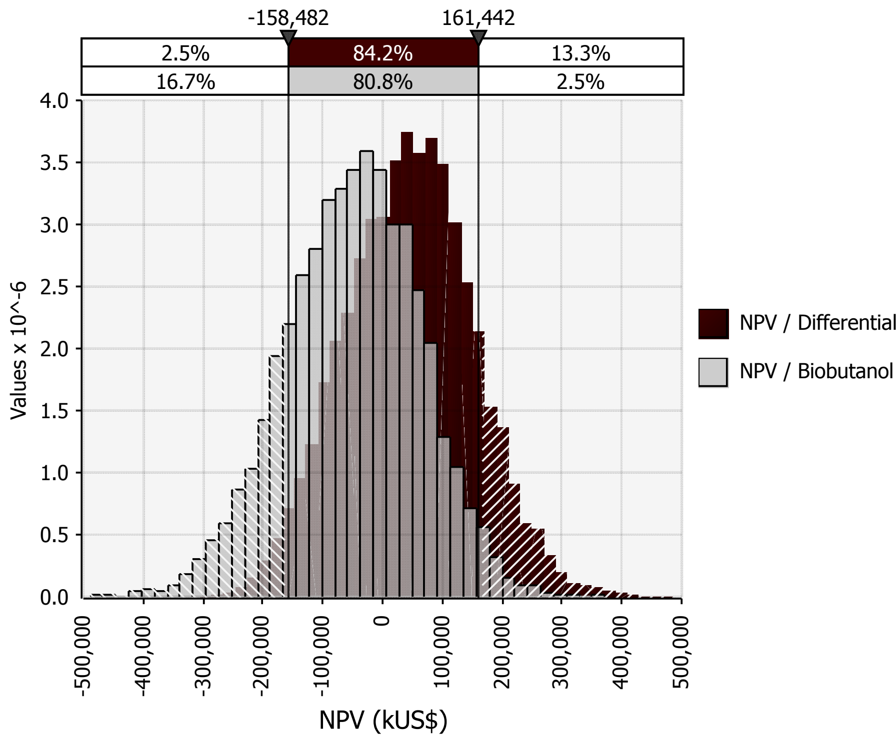


Figure 4.22 Overlapping of the NPV from the Biobutanol plant Isolated (in gray) and the Integration (in black) for Scenario A

Most of the NPV distributions are overlapped, meaning that the NPV of the biobutanol plant as an isolated venture and the biorefinery are essencially the same for most of the time.

In order to further evaluate the project potential, and according to the flowchart presented in section 4.2, the most influential variables were identified in order to further refine the scenario. Figure 4.23 shows the variables that have the biggest impact on the NPV.

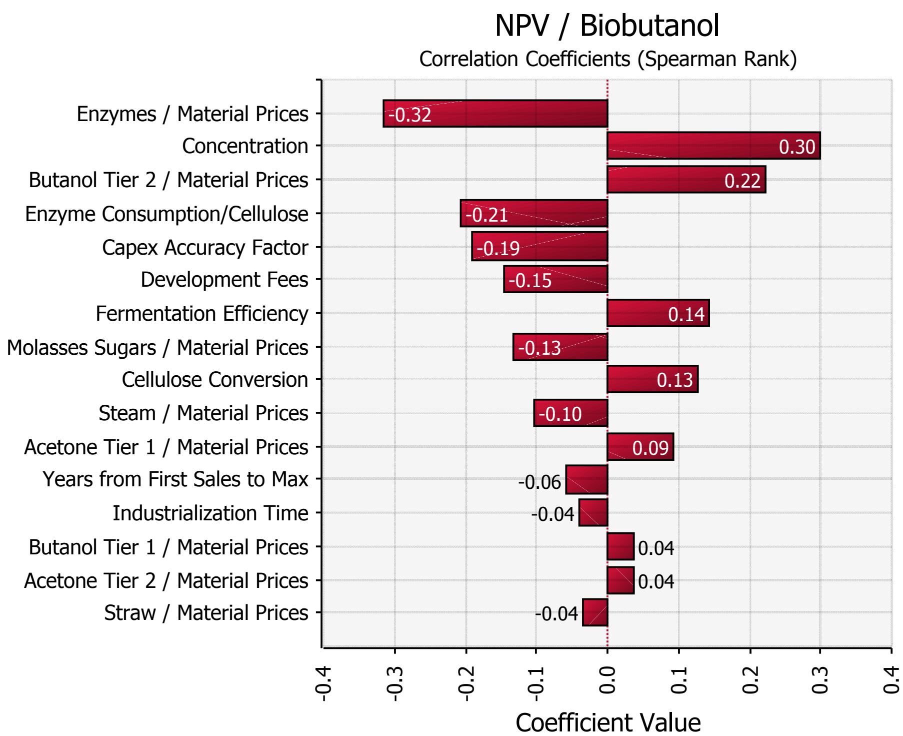


Figure 4.23 Correlation Chart for NPV in Scenario A.

As expected, butanol value and the intrinsic inaccuracy of the cost investment estimation (Capex) in such an early stage play a big role in the range obtained for NPV. Two other variables present at the top of the chart worthy of attention are enzyme price and enzyme consumption.

Enzyme costs present a big variance, as discussed in section 4.2.1.5, and the same is true for the enzyme consumption. Values for the consumption of enzyme vary greatly in literature, ranging from over 11% (Bereche, 2011) to 4% (Klein-Marcushamer, et al., 2011).

Butanol value, although very influential on NPV, was defined on historical data. To improve its distribution it would be necessary an effort from market analysts to try and figure out the range of butanol values in the future by studying markets, and demand and offer worldwide. Such an effort is unnecessary at such an early stage; a cloud graph displaying the correlation between butanol values and NPV is enough to inform how high butanol value should be to yield a positive NPV. The cloud graph is displayed in Figure 4.24.

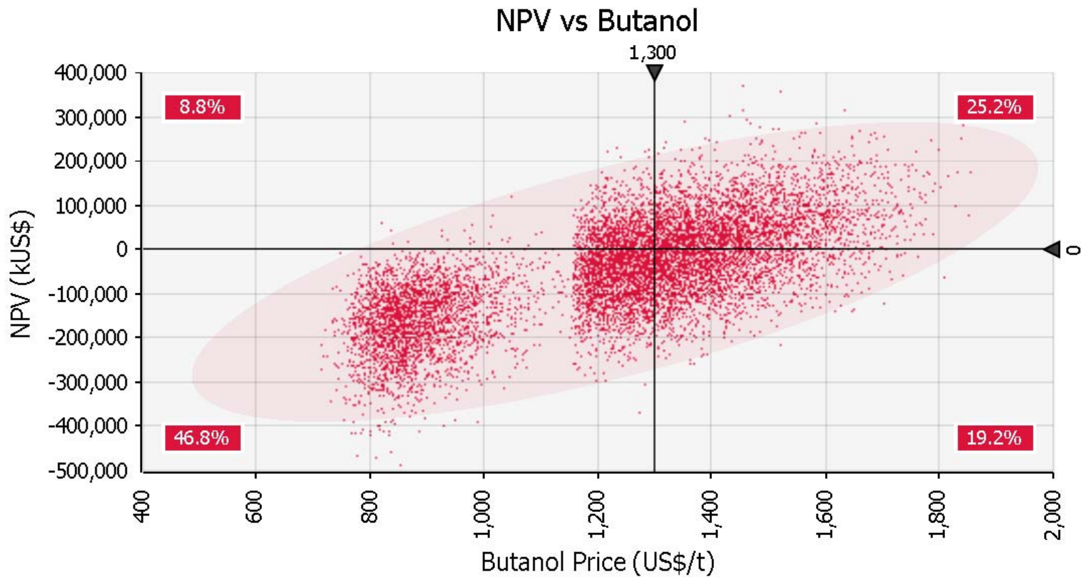


Figure 4.24 Cloud Graph for Butanol Value and NPV

The graph in Figure 4.24 shows a cloud representing all the results obtained by the Monte Carlo simulation, it is possible to observe that there are very few simulations that resulted in NPV greater than zero with butanol values under US$1300/t, specifically 8.8% of the simulations. For butanol values over US$1300/t the number of simulations that yield NPV greater than zero is close to the number of simulations that yield NPV below zero (25% above zero versus 20% below zero).

Accuracy in Capex estimation at early project stages is regularly -40% and +50%. The only way to address and reduce this range is to move further on the design of the plant, meaning that this variable cannot be improved at this point.

Solids concentration on pretreatment also showed to be an influential variable, this was defined as a discrete variable, solids concentrations defined as 5%, 10% and 15%, being 10% the concentration with highest probability of happening. This variable was not chosen for refinement in a second Monte Carlo run, but its importance in the technical development will be discussed in section 6.4.

A second Monte Carlo simulation for Scenario A was run considering smaller variations on enzyme cost and enzyme consumption. Enzyme cost was considered to have a variation between US$0.12/kg, the lowest value in the first distribution considered and US$1.25/kg, the value estimated by Klein-Marcuschamer for soy protein. According to the literature revised (see section 4.2.1.5) the values considered are very optimistic, but the economic results pointing to a negative NPV in the first Monte Carlo run justify the exercise. For enzyme consumption, a distribution between 4% and 6% over cellulose was chosen.

Table 4.9 shows the results for de second run in comparison with the first run.

Table 4.9 Comparison Between First and Second Run for the Biobutanol Plant, the Mill and the Biorefinery Economics for Scenario A

	Biobutanol Plant		Mill		Biorefinery	
	1st Run	2nd Run	1st Run	2nd Run	1st Run	2nd Run
Variable Costs (US$/t of Butanol)	1657	1034				
Variable Costs (US$/t of Sugar)			346	346	443	384
Fixed Costs (US$/t of Butanol)	59	59				
Fixed Costs (US$/t of Sugar)			8	8	13	13
Depreciation (US$/t of Butanol)	216	216				
Depreciation (US$/t of Sugar)					20	20
Investment (MUS$)	173	173			173	173
Income (US$/t of Butanol)	1893	1893				
Income (US$/t of Sugar)			535	535	646	646
Margin (US$/t of Butanol)	-40	583				
Margin (US$/t of Sugar)			181	181	169	229

Table 4.9 shows that variable costs in the second run improved significantly as expected by the reduction of the costs respective to enzyme consumption, improving also the margin. Table 4.10 shows the economic results of the second run compared to the first.

Table 4.10 Economic Results of the Second Monte Carlo Simulation run for Scenario A

	Biobutanol Plant		Integration	
	1st Run	2nd Run	1st Run	2nd Run
NPV (MUS$)	-186	62	-117	131
IRR (%)	-	0	-	0
EBITDA (MUS$)	-2	55	22	78

Due to the improvement in variable cost resulting from the reduction of enzyme consumption and reduction of enzyme price, economic results have improved significantly.

Figure 4.25 shows the NPV distribution for the second Monte Carlo simulation for the biobutanol plant.

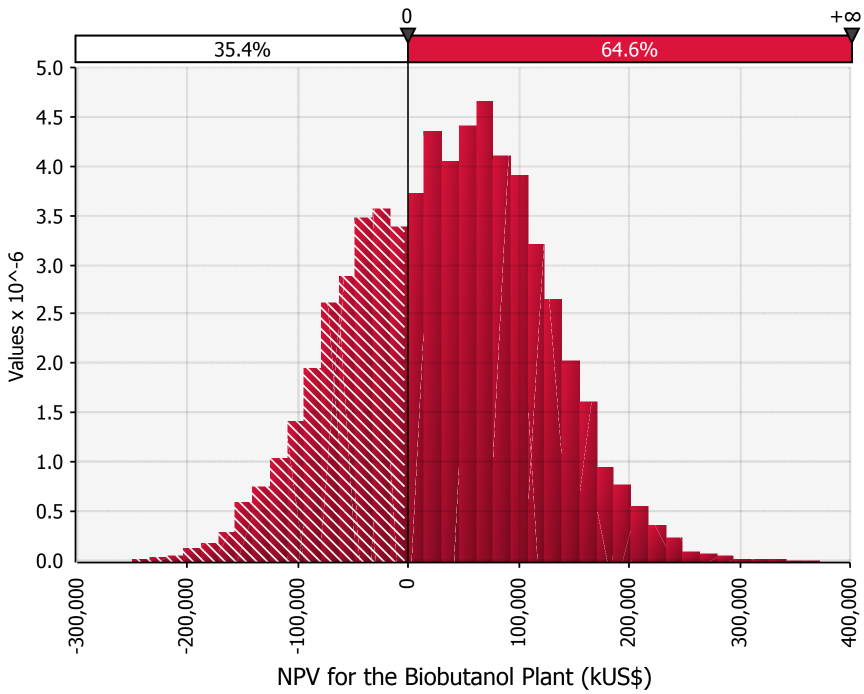


Figure 4.25 NPV Distribution for the Biobutanol Plant in the Second Monte Carlo Simulation Run of Scenario A

The distribution displayed in Figure 4.25 shows a significant improvement when compare to the distribution obtained by the first Monte Carlo simulation run (Figure 4.20). In the second run, the probability of achieving a positive NPV is increased from 34% to almost 65%.

Figure 4.26 shows the NPV for the integration of the sugarcane mill into a biorefinery configured as a biobutanol plant annex to a mill.

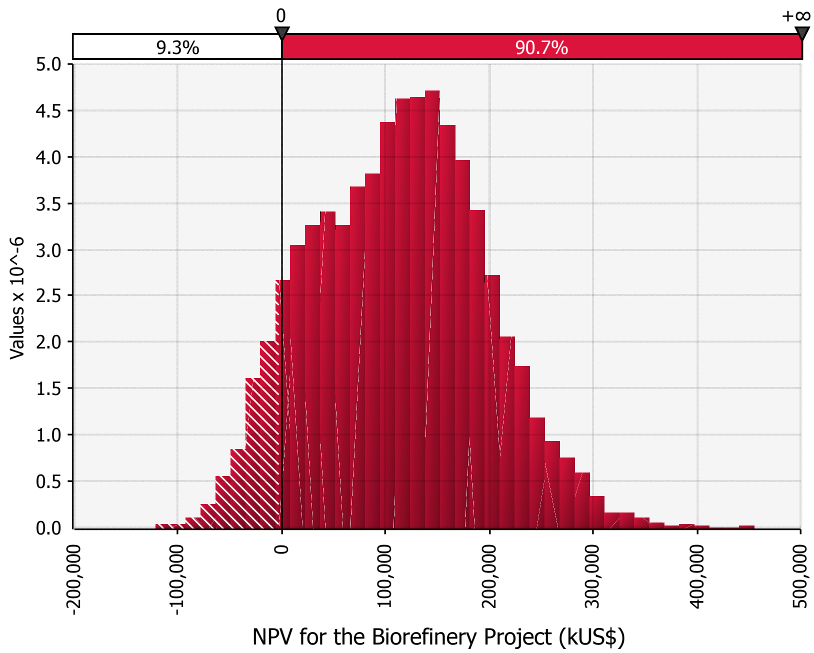


Figure 4.26 NPV for the Investment from a Sugarcane Mill to an Integrated Biorefinery in the Second Monte Carlo Simulation Run of Scenario A

When analyzing the economics of the integration of the sugarcane mill with the biobutanol plant also an improvement is observed in the second Monte Carlo simulation run when compared to the first one. The probability of achieving a positive NPV increases from around 66% to over 90%

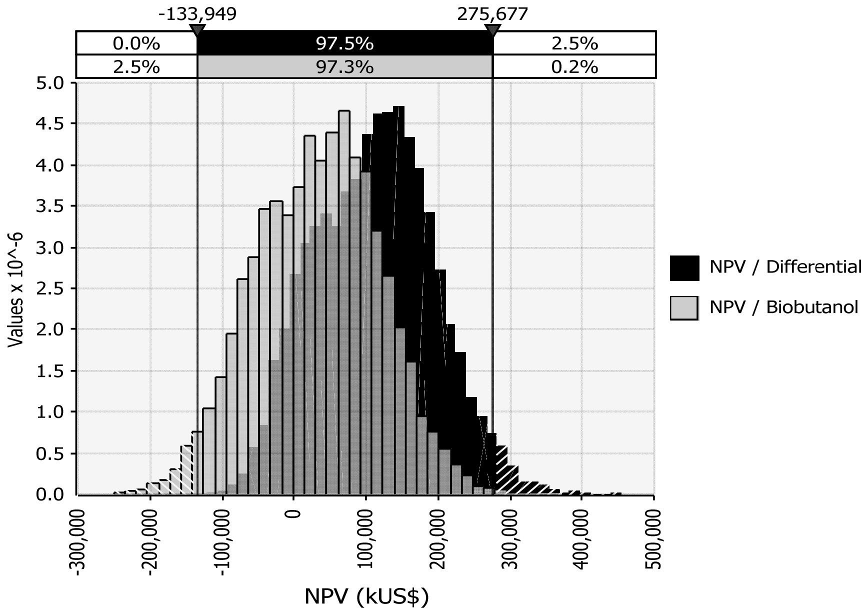


Figure 4.27 Overlapping of NPV Distributions for the Isolated Biobutanol Plant (in gray) and the Biorefinery as a Whole (in black) for the Second Monte Carlo Simulation Run of Scenario A

After the second Monte Carlo simulation run, the width of the distributions is still large, but there is an important improvement in the probability of the project achieving a positive NPV value, which means a return over investment higher than the discount rate used for the project evaluation, which in this work is around 11%. The width of the distributions shows that an economic metric of the project can be greatly affected by the uncertainties of the inputs, reinforcing the necessity of using distributions instead of fixed values in early stage project assessment.

Figure 4.28 shows the main variables impacting on NPV.

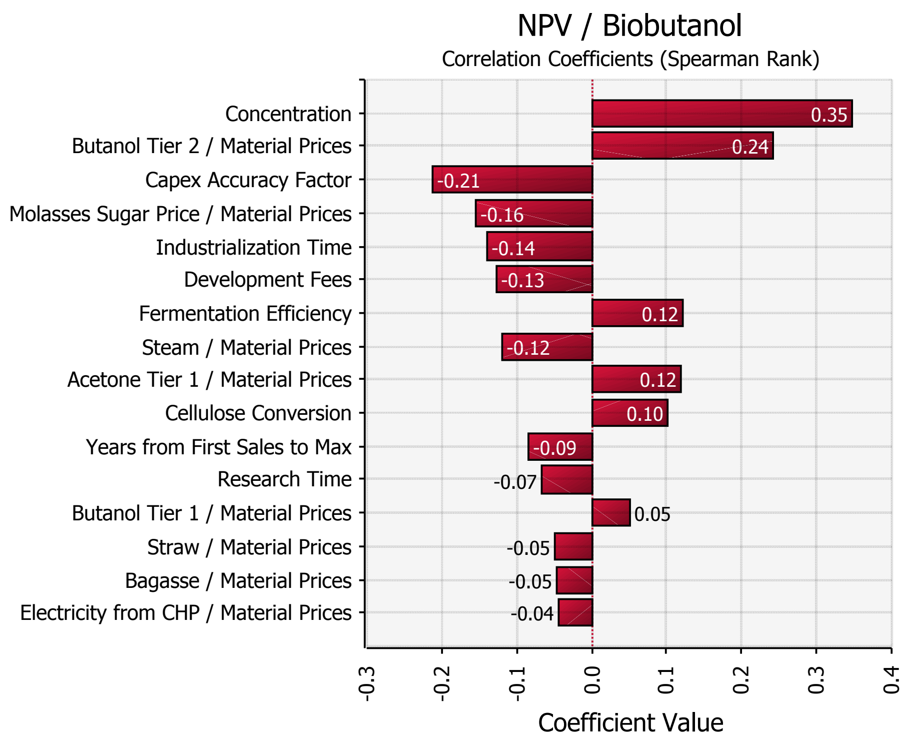


Figure 4.28 Correlation Graph for the Second Monte Carlo Simulation Run of Scenario A

As shown in the correlations graph presented in Figure 4.28, enzyme consumption and enzyme price ceased to be influential variables on NPV on the second Monte Carlo run, or better, ceased to be a source of uncertainty since its value is much more restricted in this second analysis. Variables connected to raw materials, products and investment (Capex accuracy and solids concentration in pretreatment), are now presented as most influential, indicating that, should the project continue its development, resources should be driven to raw material sourcing, market assessment of renewable biobutanol and pretreatment development. Enzyme pricing and efficiency of consumption is also an area of concern and of course an important quantity of resources should be directed to it.

4.2.3.2. Scenario B

Scenario B was analyzed in the same way as scenario A, as explained in section 4.2 scenario A has a bigger scale than scenario B, meaning that it is expected that the economic results of scenario B will be worse than those obtained for scenario A.

In spite of this expected difference in result, the analysis of scenario B is important due to the fact that there are many sugarcane mills in Brazil with crushing capacity around 3.5 million tons of sugarcane per year, whereas there is a very small amount of mills that have a 9 million tons of sugarcane per year crushing capacity, if indeed there is any. Because of this, scenario B is a much more realistic scenario for Brazilian mills.

Table 4.11 displays the costs and incomes for the biobutanol plant, for the mill prior to the integration and for the whole biorefinery in scenario B, the costs and incomes for the biobutanol plant are calculated having as basis the biobutanol production, whereas the costs and incomes for the mill prior to integration and the biorefinery are calculated in the sugar production basis. Using the sugar production as basis for the mill and the biorefinery makes it easier to make a comparison of the results of the mill before and after the integration.

Table 4.11 Comparison Between the Biobutanol Plant, the Mill and the Biorefinery Costs and Incomes for Scenario B

	Biobutanol Plant	Mill	Biorefinery
Variable Costs (US$/t of Butanol)	1676		
Variable Costs (US$/t of Sugar)		346	441
Fixed Costs (US$/t of Butanol)	133		
Fixed Costs (US$/t of Sugar)		20	32
Depreciation (US$/t of Butanol)	393		
Depreciation (US$/t of Sugar)			36
Investment (MUS$)	118		118
Income (US$/t of Butanol)	1893		
Income (US$/t of Sugar)		535	643
Margin (US$/t of Butanol)	-309		
Margin (US$/t of Sugar)		169	133

Costs are increased for the biorefinery when compared to the mill, and a depreciation cost is added due to the assets of the biobutanol plant, income is also increased, indicating that the reduction in income due to the reduction of electricity export is compensated by the added incomes from butanol, acetone and ethanol.

Table 4.12 displays the economic results of the scenario B.

Table 4.12 Economic Results for Scenario B

	Biobutanol Plant	Integration
NPV (MUS$)	-89	-56
IRR (%)	-	-
EBITDA (MUS$)	-2.9	6.2

In the same way as in the scenario A, a look into the results of the economic analysis would lead to classifying the project as not economically feasible, to further understand the economic results, risk analysis was performed.

Figure 4.29 shows the distribution obtained for the net present value for the biobutanol plant in scenario B.

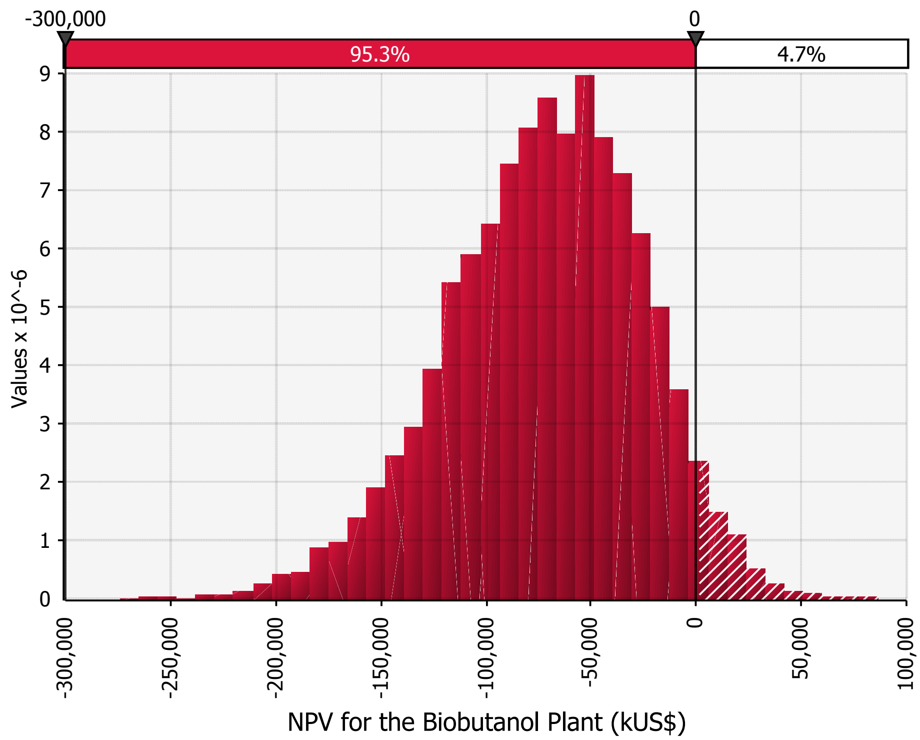


Figure 4.29 NPV Distribution for the Biobutanol Plant in Scenario B

The distribution displayed in Figure 4.29 shows that there is a very little probability (4.7%) of the biobutanol plant project achieving a positive NPV in the current configuration.

Similarly to the analysis in scenario A, when seen by the perspective of the integration of the mill, the economic results presents better results due to pricing power of the utilities supplied to the butanol plant versus the value of electricity in the market. Figure 4.30 shows the distribution of the net present value obtained for the integration of the mill into a biorefinery.

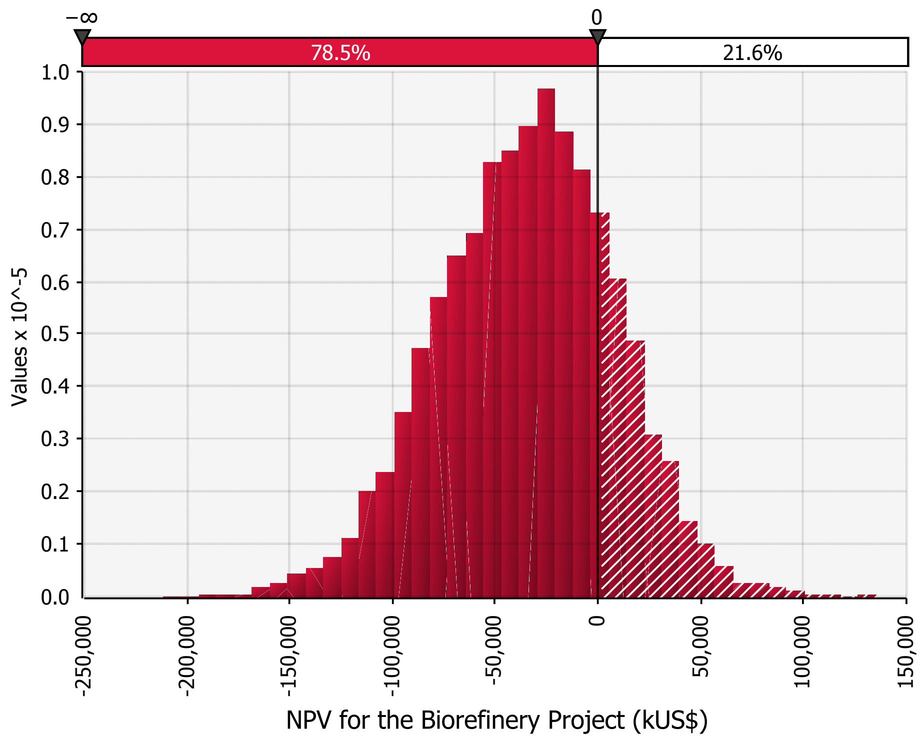


Figure 4.30 NPV Distribution for the Integration of the Mill into a Biorefinery for Scenario B

Correlations to the variables with the biggest impacts on the economic results were identified; Figure 4.31 displays the variables with the biggest correlations to the net present value in decreasing order.

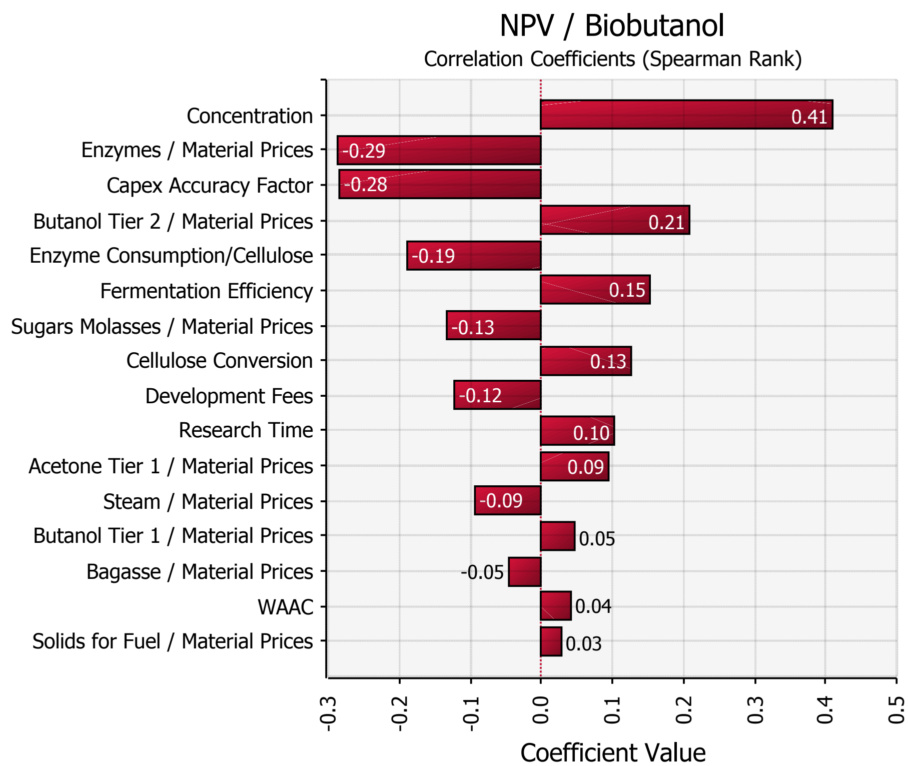


Figure 4.31 Correlation Graph for the NPV of the Biobutanol Plant in Scenario B

Similarly to scenario A, the variables with the greatest correlations to the net present value were related to investment (concentration of solids in pretreatment, capex accuracy), to product value, to raw material cost and conversion and enzyme cost.

As explained for scenario A in section 4.2.3.1 enzyme price and consumption efficiency (in % over cellulose) are the only variables that could be refined at an early stage of a project. The same enzyme price and consumption distributions used for the second Monte Carlo simulation run in scenario A was used for the second Monte Carlo simulation run in scenario B.

Table 4.13 shows the comparison between the results of the first and second Monte Carlo simulation runs. It is possible to observe an important reduction in the variable cost due to the reduction of cost with enzyme. As a consequence, an increase in the product margin is observed.

Table 4.13 Comparison Between the Results for the First and Second Simulations for Scenario B

	Biobutanol Plant		Mill		Biorefinery	
	1st Run	2nd Run	1st Run	2nd Run	1st Run	2nd Run
Variable Costs (US$/t of Butanol)	1676.0	1052.9				
Variable Costs (US$/t of Sugar)			345.8	345.8	440.7	383.2
Fixed Costs (US$/t of Butanol)	133.0	133.0				
Fixed Costs (US$/t of Sugar)			20.1	20.1	32.4	32.4
Depreciation (US$/t of Butanol)	392.7	392.7				
Depreciation (US$/t of Sugar)					36.2	36.2
Investment (MUS$)	118.2	118.2			118.2	118.2
Income (US$/t of Butanol)	1892.6	1892.6				
Income (US$/t of Sugar)			535.0	535.0	642.5	642.5
Margin (US$/t of Butanol)	-309.1	314.0				
Margin (US$/t of Sugar)			169.0	169.0	133.2	190.7

Table 4.14 shows the economic results for the first and second simulations, in the economic results it is also possible to observe an important improvement. Both in the case of the biobutanol plant and in the mill integration, the EBITDA (Earnings before Interest, Tax, Depreciation and Amortization) which represents the operational profit of the plant became positive. When analyzing the project from the point of view of the integration of the mill into the biorefinery, it is even possible to have a positive internal rate of return (IRR).

Table 4.14 Comparison between the Economic Results for the First and Second Simulations for Scenario B

	Biobutanol Plant		Integration	
	1st Run	2nd Run	1st Run	2nd Run
NPV (MUS$)	-89	-18	-56	18
IRR (%)	-	1%	-	10%
EBITDA (MUS$)	-2.9	53.3	6.2	76.3

The distributions of the net present value also showed improvements in the probability of the project yielding a positive NPV, whereas in the first Monte Carlo simulation the probability of achieving a positive NPV was around 5%, in the second Monte Carlo simulation its probability increased to 25%. Figure 4.32 shows the distribution of the net present value for the second Monte Carlo run.

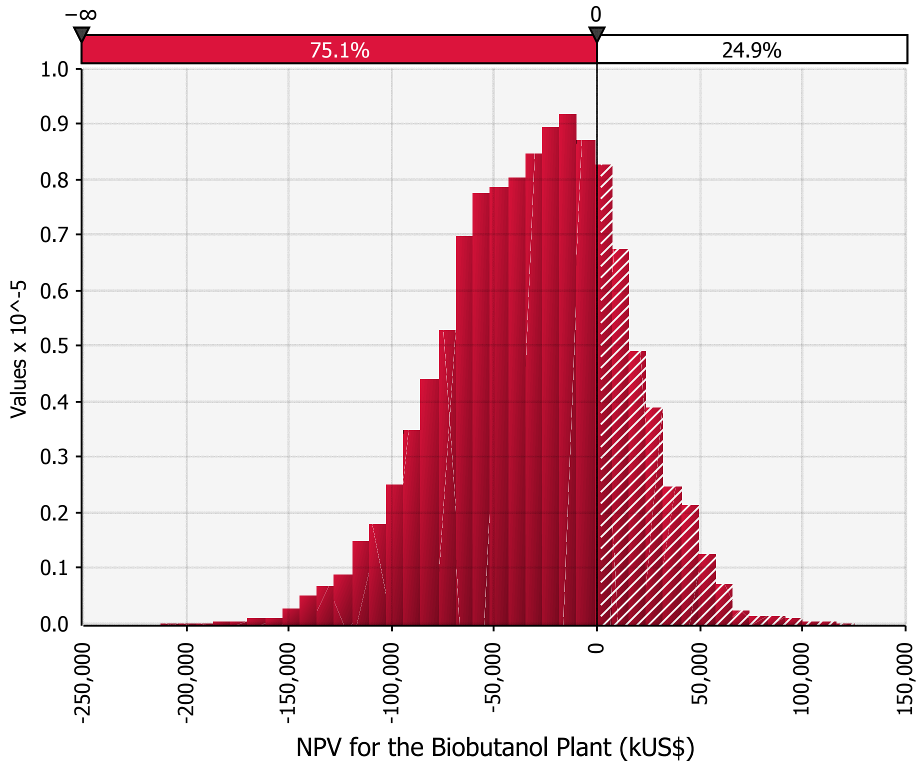


Figure 4.32 NPV Distribution in the Second Monte Carlo Simulation for Scenario B

As in the cases analyzed previously, in this second simulation of Scenario B the economic results were better when the project was observed from the point of view of the integration of the sugarcane mill to a biobutanol plant to form a biorefinery instead of the isolated biobutanol plant. An important improvement in the probability of achieving a positive net present value was also observed in comparison to the first Monte Carlo simulation run, in the second Monte Carlo simulation, the probability of a positive NPV being achieved became 57% whereas in the first Monte Carlo simulation the probability was around 20%

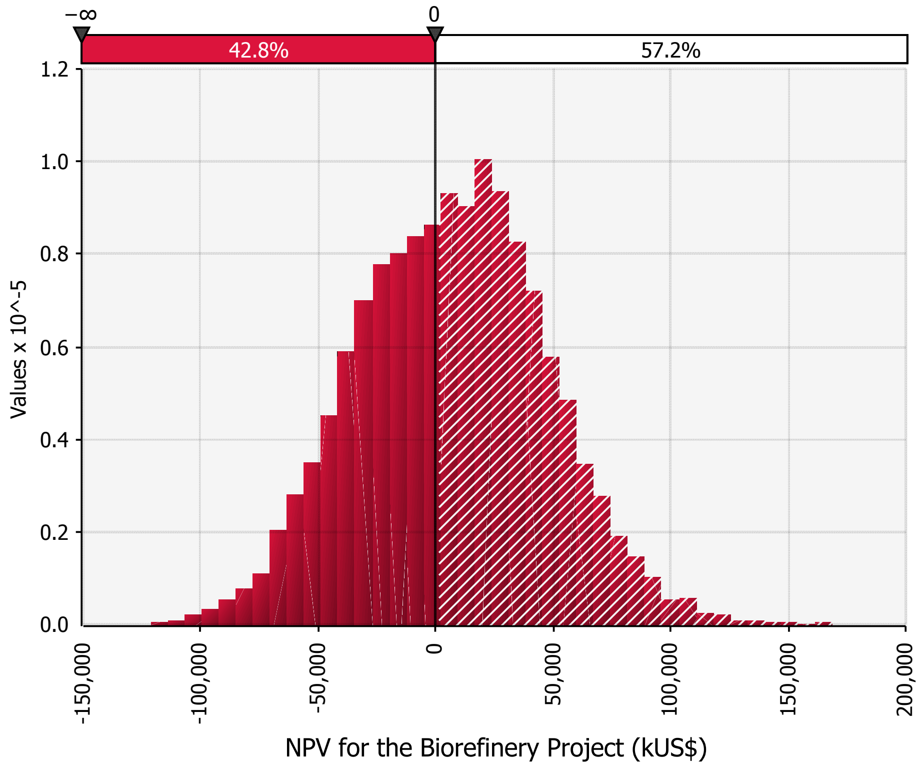


Figure 4.33 NPV Distribution for the Integration of a Sugarcane Mill into a Biorefinery for the Second Monte Carlo Run in Scenario B

As with the first Monte Carlo simulation run, the correlations between the variables and the economic result were calculated and the variables with the highest impacts were organized in a graph. Figure 4.34 shows that the enzyme price and consumption dropped in importance on the list since its uncertainties were reduced from the first run to the second, but especially because of the difference in the economic results in the two runs enzyme price and enzyme efficiency in hydrolysis should remain one of the main areas to concentrate project resources. The risk analysis also points to other variables as important in project development such as concentration of solids in pretreatment, capex estimation, butanol market price, price of molasses used as fermentation media complement, fees that the project might have to pay to technology developers and cost with steam.

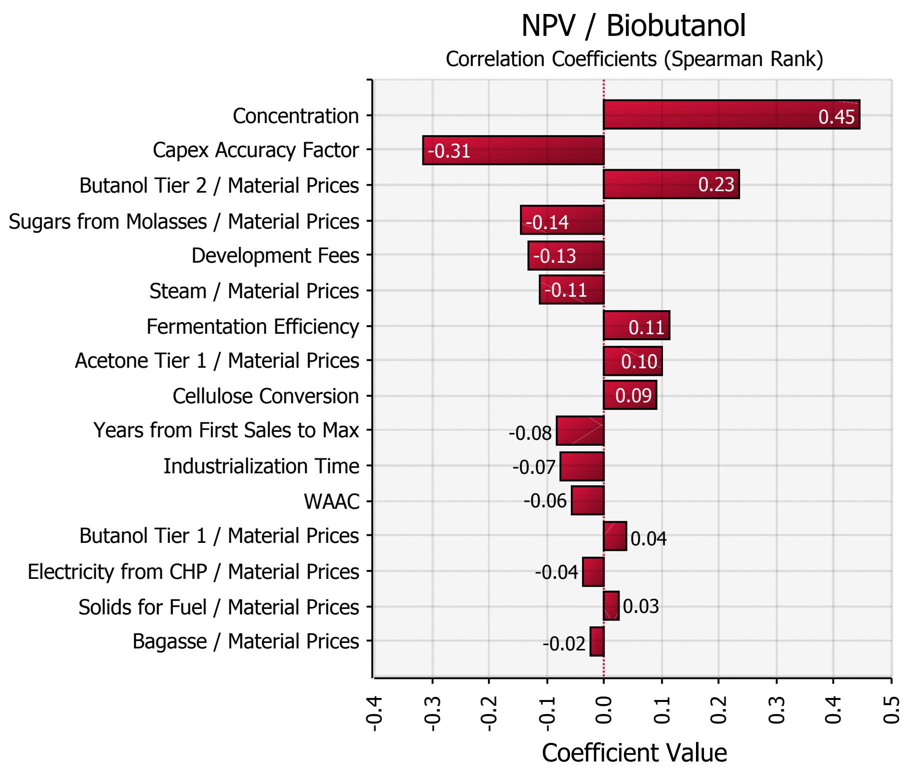


Figure 4.34 Correlation Graph for the NPV in the Second Monte Carlo Run for Scenario B

4.2.4. Building a Project Development Plan around the Risk Analysis Results;

It is possible to use the correlation graphs to help in the planning the next steps in the development of a project. The variables with highest correlation to the targeted economic index indicate where to allocate resources; these variables have a high probability of leveraging the economic feasibility of a project or being the main reason for stopping the project.

As the correlation graphs shows in all scenarios, butanol price is a variable that influence greatly on NPV, indicating that marketing efforts to improve foresight on product prices would be needed in the next phases of the project.

Enzyme price is another variable with high correlation with NPV, meaning that determining the correct enzyme price with the vendors is an important step in building the business plan.

In planning the technical development, enzyme consumption and solids concentration in pretreatment have much higher correlation to attractive economic results than fermentation variables such as fermentation yield or titer. This information is important to the project team in defining research and development budgets, personnel hiring and development schedules. Although research and development efforts will be needed in all process steps, the risk analysis indicates that pretreatment and hydrolysis are the processes that brings the highest risks and highest leverages for the project feasibility. This information indicates that more resources should be directed into pretreatment and hydrolysis development, especially the aspects of solids concentration and enzyme consumption.

Another important variable appearing in the risk analysis of all scenarios and runs is the butanol price, it is expected that the product price will play an important role in the business plan, so marketing efforts to predict as best as possible the future market should be one of the priorities in resource allocation.

The intrinsic imprecision of the investment estimative used in this work also played a major role in the economic results distributions, for an early stage assessment, methodologies such as the process step score, or even educated guesses could help form a scenario that is both acceptable in terms of precision and time consumption. As the project progresses tough, it is important that such estimates be replaced by better estimates in Order of Magnitude using the traditional engineering estimates, being that estimation methodologies such as the process step score, although practical, could lead to mistakes as explained in section 2.3.1.

4.2.5. Applying a Risk Analysis to the Biobutanol Case using a Low Level of Detail.

The production of biobutanol from sugars is thoroughly described in the literature as it is possible to verify in this chapter, this means that there is much more information available of such process than the early stage analysis methodology proposed in this work demands. The reduction in detail of the process description might lead to economic and risk results that are different from the original analysis, but shouldn´t lead to fundamentally different conclusions. Also, a less detailed process analysis should ideally yield a more promising result than a more detailed one, as to guarantee that an economically feasible project won´t be discarded in its beginning because of the early stage analysis being too conservative.

In order to confirm that an early stage analysis with small amount of information would yield results to drive a decision maker in a similar direction than the more detailed analysis did, an exercise based on the biobutanol case was done.

The process described in this chapter and used for the risk analysis was simplified to a group of general information that describes the whole process. This aims to mimic the kind of information that would be available at early stages of a project and thus the kind of information that would be used for an early stage economic risk analysis.

Table 4.15 shows a set of process data that broadly describes the biobutanol process in a condition similar to Scenario A evaluated in section 4.2.3.1.

Table 4.15 Process Parameters for the Biobutanol Process

Process Data	
Steam Consumption (t/t wet biomass)	0.55
Sugar Yield on Biomass (t Sugars/ t of dry biomass)	43.76%
Solids Concentration (%)	14%
Enzyme Consumption (% Over Biomass)	0.62%
Yield on Butanol (t Butanol/ t of Sugars)	0.219
Steam Consumption in Distillation (t/t Butanol)	10.90
Acetone Butanol Ratio (t Acetone/ t of Butanol)	0.506

A block diagram of the process can be seen in Figure 4.35.

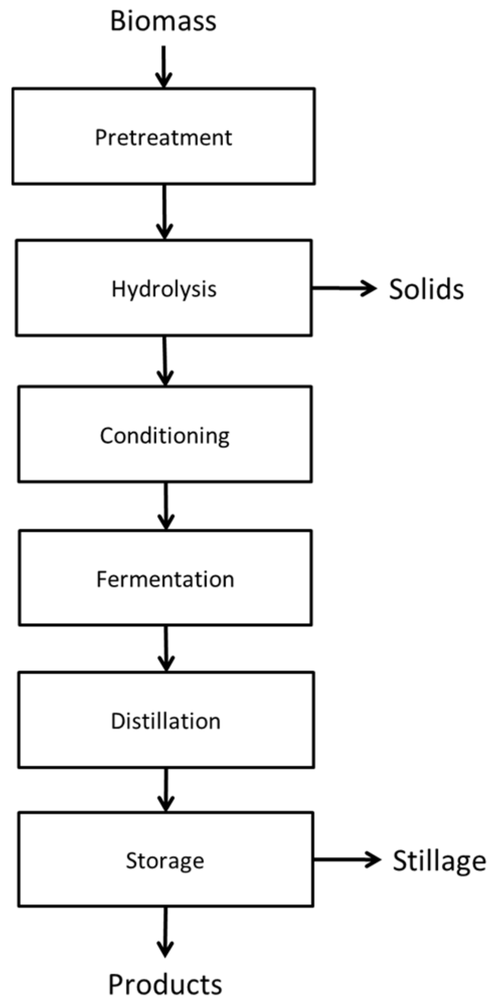


Figure 4.35 Block Diagram of the Biobutanol Process

The result of the economic analysis is shown in Table 4.16.

Table 4.16 Economic Results

Economic Results	
Variable Costs (US$/t)	1,515
Fixed Costs (US$/t)	56
Investment (MUS$)	155
Full Manufacturing Cost (US$/t)	1,176
NPV (MUS$)	-54.8
IRR (%)	-

The deterministic economic analysis results show a negative NPV indicating that the biobutanol project is not feasible. A risk analysis was performed and distributions were assigned to the process variables presented in Table 4.15 and the prices of raw materials, utilities and products.

The distributions were assigned according to the recommendations in section 2.4.3 and Figure 2.14. For the biobutanol and acetone prices uniform distributions were assigned instead of the distributions found in sections 4.2.1.1 and 4.2.1.2.

Table 4.17 shows the distributions assigned to the inputs and the maximum, minimum and modal values of the distributions.

Table 4.17 Input Distributions for the Economic Risk Preliminary Analysis

Name	Distribution	Min	Mode	Max
Acetone Price (US$/t)	Normal	752	900	1048
Biomass Price (US$/t)	Normal	21	25	29
Butanol Price (US$/t)	Normal	1086	1300	1514
Effluent Cost (US$/t)	Normal	0.84	1.00	1.16
Electricity Price (US$/MWh)	Normal	54	65	76
Enzyme Consumption (% Over Biomass)	Triangular	0.41%	0.54%	0.63%
Enzyme Price (US$/t)	Triangular	2392	7140	10463
Ethanol Price (US$/t)	Normal	543	650	757
Molasses Sugar Price (US$/t)	Normal	230	275	320
Solids Price (US$/t)	Normal	21	25	29
Solids Concentration (%)	Triangular	5%	14.4%	20%
Steam Price(US$/t)	Normal	14	16	19
Steam Consumption (t/t wet biomass)	Normal	0.46	0.55	0.64
Steam Consumption in Distillation (t/t Butanol)	Normal	9.1	10.9	12.7
Sulphur Price (US$/t)	Normal	125	150	175
Water Price (US$/t)	Normal	0.8	1.0	1.2
Yield on Biomass (t Sugars/ t of dry biomass)	Normal	0.37	0.44	0.51
Yield on Butanol (t Butanol/ t of Sugars)	Normal	0.18	0.22	0.26
Capex Accuracy Factor	Triangular	0.6	1	1.5

The NPV distribution output of the risk analysis indicates that there is an approximately 54% chance of the project achieving an NPV greater than zero, this result is more optimistic than the one presented in Figure 4.20, which was around 34%, the reason is the simpler process model deriving from a smaller set of information. A simpler process model means that utility consumptions are underestimated, the same being true for raw materials and chemicals used in the process, also, a simpler model will yield through the Process Step Scoring method a smaller investment due to the absence of process steps such as solid/liquid separations and smaller throughput that is a result of a less detailed mass balance.

The NPV distribution is shown in Figure 4.36.

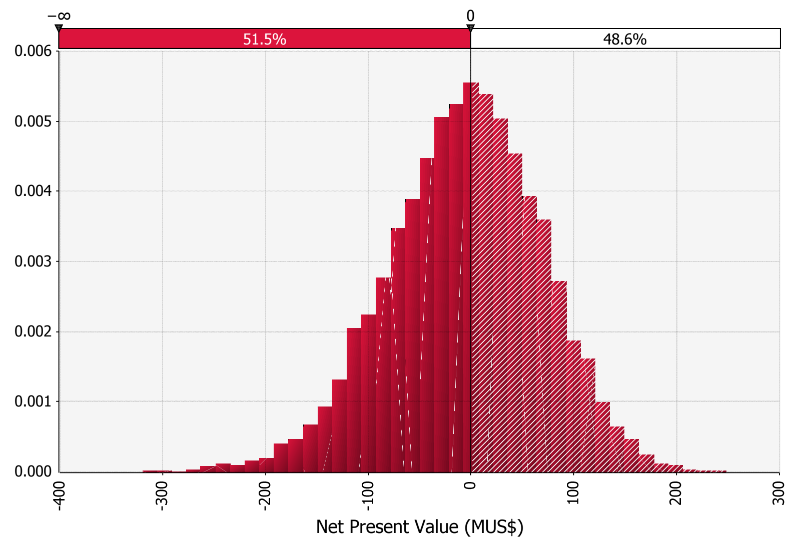


Figure 4.36 NPV Result Distribution for the Preliminary Risk Analysis for the Biobutanol Project.

The correlations found between the inputs and the NPV show that enzyme price, butanol price, process yields, investment estimation accuracy, enzyme consumption and solids concentration in hydrolysis are the most influential variables in the risk analysis. This result is consistent with the more detailed analysis presented in this chapter.

The correlations between inputs and NPV are shown in Figure 4.37.

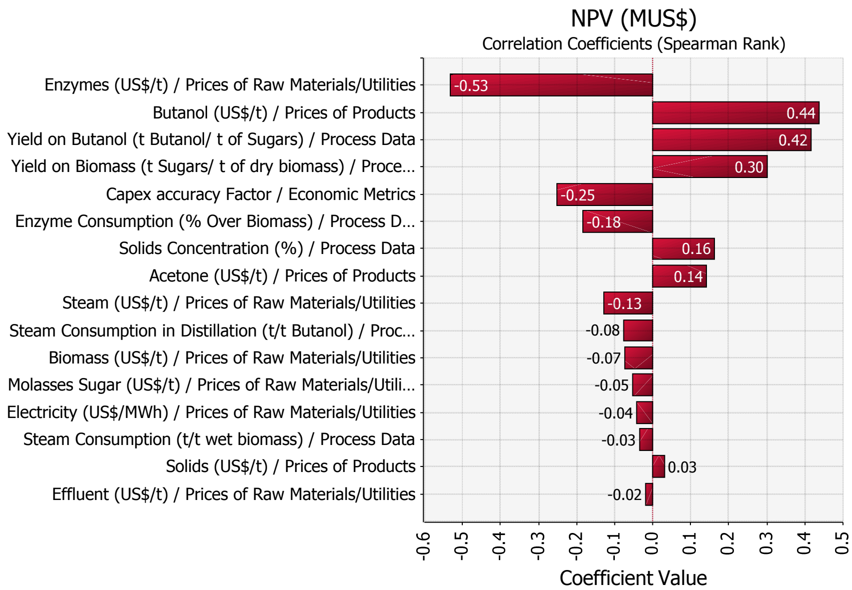


Figure 4.37 Main Influences in the Biobutanol Project Detected in the Preliminary Analysis

The results of the risk analysis show that the methodology presented, although presenting the uncertainties of the economic analysis, did not yield lower probabilities of a desired economic result than the more detailed analysis, on the contrary, the results of the less detailed analysis showed a better probability of achievement of a NPV greater than zero. This is an important feature of this methodology; an earlier and less detailed analysis yields a more optimistic result than a more detailed one, which is desirable, so there would be no risk of a feasible project being stopped because of an excessively pessimistic early stage analysis. Also, it is important to note that the less detailed and the more detailed analysis pointed out to the same conclusion that the project is indeed economically challenging.

Both analysis showed similar results regarding the correlations between the inputs and NPV, they pointed out generally to the same inputs as being the most influential in the economic results of the project, those being: enzyme price, butanol price, process yields, investment accuracy and solids concentration on hydrolysis. This result shows that stochastic risk analysis can be used as an aid in development from the very start of the project.

5. CHAPTER 5: BASE CASE II DEVELOPMENT: MUCONIC ACID

5.1. General

The process to produce butanol from ABE is very well described in the literature, in such a way that it was possible to make flowsheets and fairly detailed mass and energy balances as seen on Chapter 4. The level of detail presented for the butanol analysis is not required by the method, i.e. economic and risk analysis can be run with much less information.

To better exemplify the applicability of the methodology a second case was chosen to analyze a project in which the process is less known. In this second case, a process not quite familiar was evaluated: the manufacture of muconic acid from biomass. The transformation process to produce sugars from biomass was based on the work of Bereche (2011), as in the biobutanol case, fermentation was based on a patent filed by the company Myriant (2013) in which a purification by crystallization is also suggested. A block diagram to represent the process studied is shown in Figure 5.1.

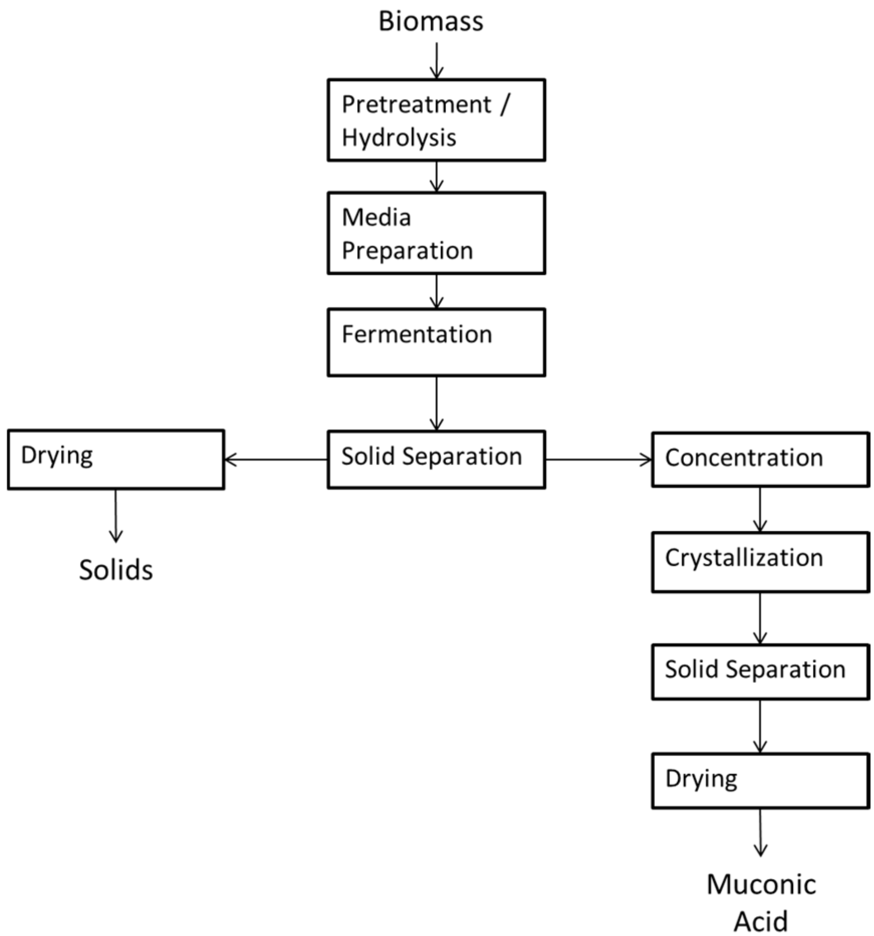


Figure 5.1 Muconic Acid Manufacture Block Diagram

Muconic acid is produced through sugar fermentation and purified through concentration of the fermentation media and crystallization of the muconic acid, production process is finalized by a drying step to yield the final product.

A genetically modified *E. coli* is used to transform sugars into muconic acid, fermentation starts with a 2.5% w/w solution of sugars and yields a titer of 1.6% w/w of muconic acid. Fermentation time is 48h and temperature is 37°C (Myriant, 2013).

Because detail in process information for the muconic acid production is scarce, the risk analysis should consider the imprecisions of the inputs to be large, as shown in the next section.

5.2. Inputs and Premises

One of the applications suggested for Muconic Acid is as a precursor for Adipic Acid production, which in turn is an intermediate for nylon (Xinxiao, et al., 2013). Muconic acid is not a commonly marketed chemical, especially in bulk, so historical data on its price is not readily available. Adipic acid on the other hand, is a commonly traded chemical, so price history is available (AliceWeb, 2015). In this analysis, the adipic acid price distribution was considered (Figure 5.2), and muconic acid price was defined to be 70% of that of adipic acid and a normal distribution was assigned (Figure 5.3).

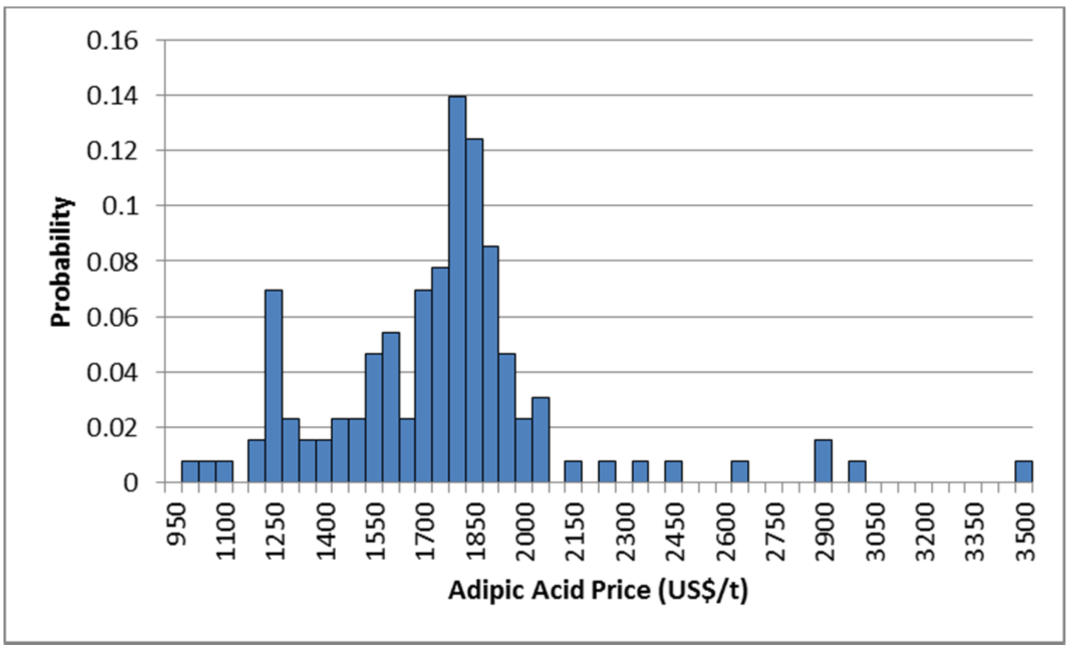


Figure 5.2 Adipic Acid Price Distribution (AliceWeb, 2015).

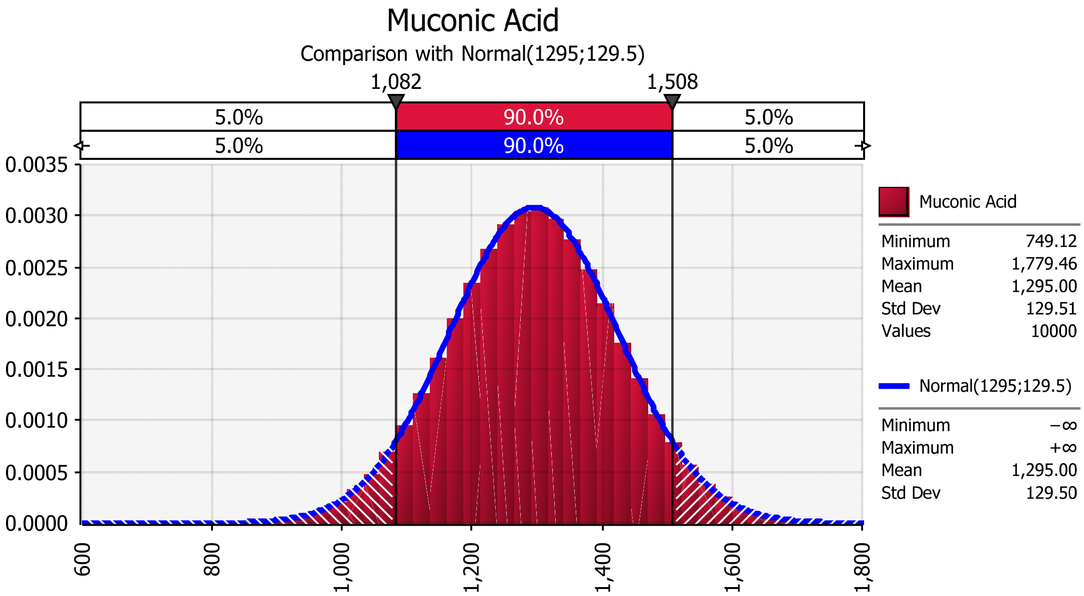


Figure 5.3 Distribution for Muconic Acid Price (US$/t)

Table 5.1 summarizes the inputs for the economic and risk analysis of the muconic acid case, for each variable, the type of distribution, the maximum and minimum and mean value are displayed.

Table 5.1 Inputs for Economic Model and Risk Analysis

Name	Distribution	Min	Mean	Max
Research Time	Discrete	2	3	4
Industrialization Time	Discrete	2	3	4
Years from First Sales to Max	Discrete	2	3	4
Straw	Normal	18.6	30.0	41.3
Enzymes	Triangular	173.5	7173.3	11199.1
Electricity	Normal	39.6	65.0	92.6
Steam	Normal	6.6	12.0	17.2
Muconic Acid Price	Normal	722	1250.0	2624.9
Research Cost	Normal	315.9	600.0	834.5
Development Fees	Discrete	2%	5%	10%
Temperature	Normal	114.0	190.0	272.5
Hemicellulose Removal	Triangular	63%	70%	77%
Cellulose Removal	Triangular	4%	4%	5%
Steam Consumption	Normal	0.33	0.55	0.76
Cellulose Conversion	Triangular	62%	69%	76%
Hemicellulose Conversion	Triangular	40%	49%	60%
Hydrolysis Concentration	Discrete	5%	10%	15%
Enzyme Consumption	Triangular	4%	9%	11%
Yield	Normal	38.04%	64.00%	87.92%
MA Concentration	Triangular	1.20%	1.77%	2.49%
Final Concentration	Normal	32%	55%	76%
Saturation Concentration	Normal	35%	60%	82%

5.3. Mass and Energy Balance

A mass and energy balance was built according to the flowsheet displayed in Figure 5.1 and the technical information in the literature used for pretreatment and hydrolysis process (Bereche, 2011) and fermentation (Myriant, 2013). For the process steps not described in either document, i.e. separation, rule of thumb design was used based on the product properties. A crystallization process followed by drying was imagined for the muconic acid purification based on the fact that muconic acid is a crystal in ambient temperature. Table 5.2 displays the rates of consumption of raw material and utilities in the muconic acid manufacturing process.

Table 5.2 Muconic Acid Plant Consumptions of Materials and Utilities

Material / Utility	Consumption
Straw (t/h)	30.0
Enzymes (t/h)	1.3
Water (t)	302.9
Electricity (MW)	4.1
Steam (t/h)	61.8
Effluent Treatment (t/h)	3.2

Table 5.3 displays the muconic acid hour production and the production of the by-product which are solids derived from biomass that should be destined for energy production.

Table 5.3 Muconic Acid Plant Production

Product	Production
Muconic Acid (t/h)	5.0
Solids Fuel (t/h)	20.7

Table 5.4 displays the specific consumptions of raw material and utilities for the muconic acid manufacturing process.

Table 5.4 Specific Consumptions of Materials and Utilities in the Muconic Acid Plant

Material / Utility	Consumption
Straw (t/t)	6.0
Enzymes (t/t)	0.3
Water (t/t)	60.6
Electricity (MW/t)	0.8
Steam (t/t)	12.4
Effluent Treatment (t/t)	0.6

5.4. Economic and Risk Analysis

Economic analysis was done based on the mass and energy balance for the muconic acid production plant, Table 5.5 shows the main economic parameters used for the construction of the cash flow of the project and the economic calculations, Table 5.6 shows the main costs calculated for muconic acid production.

Table 5.5 Economic Inputs or the Muconic Acid Plant Project

Capacity (kt/y)	40
Operating Time (h/y)	8000
WAAC (%)	11%
Research Time (y)	3
Industrialization Time (Y)	3
Years from First Sales to Max (Y)	3
Research Cost	600

Table 5.6 Muconic Acid Plant Production Costs

Costs	
Variable (USS/t Muconic Acid)	3194
Fixed (US$/t Muconic Acid)	86
Investment (MUS$)	93
Depreciation (US$/t Muconic Acid)	233
FMC (US$/t Muconic Acid)	3513
Raw Materials (US$/t Muconic Acid)	180
Enzymes (US$/t Muconic Acid)	2681
Utilities (US$/t Muconic Acid)	263
Margin (US$/t Muconic Acid)	-2114

It is possible to identify readily in Table 5.6 that the full manufacturing cost (FMC) of muconic acid is much higher than the value estimated for its market as an adipic acid precursor. This consideration is enough to conclude that the project to produce muconic acid from biomass, in this specific configuration is not economically feasible. Risk analysis also shows that the probability of achieving a positive margin for this product is around 8%. Figure 5.4 shows the distribution obtained for the product margin. The product margin was chosen as the economic result to be analyzed in this case due to the very high full manufacturing cost when compared to the product price, in this case, using the NPV as economic metric would be pointless because of the fact that the the whole distribution of NPV values would be negative.

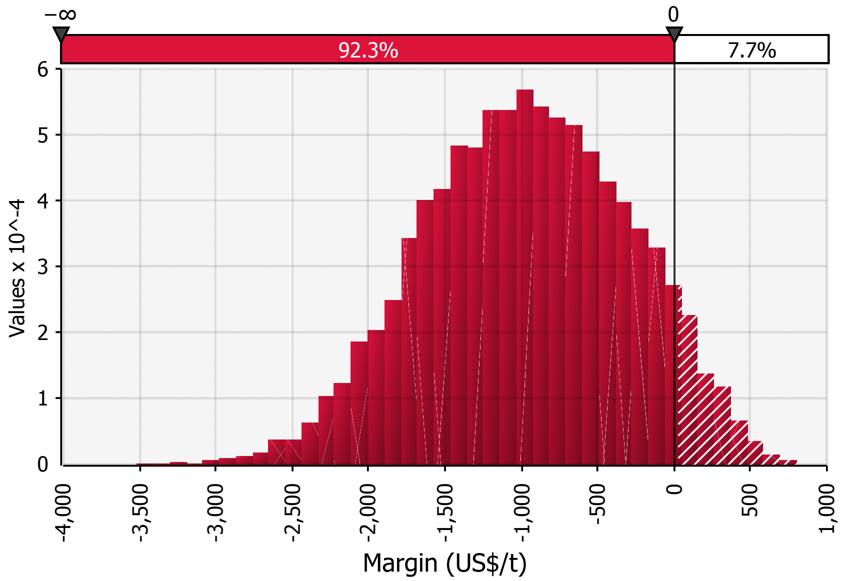


Figure 5.4 Distribution of the Product Margin for Muconic Acid Manufacturing from Biomass

The results presented in Figure 5.4 and Table 5.6 shows that the muconic acid process is not feasible, the risk analysis also provides the correlation between the variables used in the model and the output, in this case, the product margin. Figure 5.5 presents a correlation graph displaying the variables with the highest impact in the product margin in decreasing of importance. From this graph, it is possible to identify the main inputs to which a refining effort should be applied in order to confirm the non-feasibility of the process.

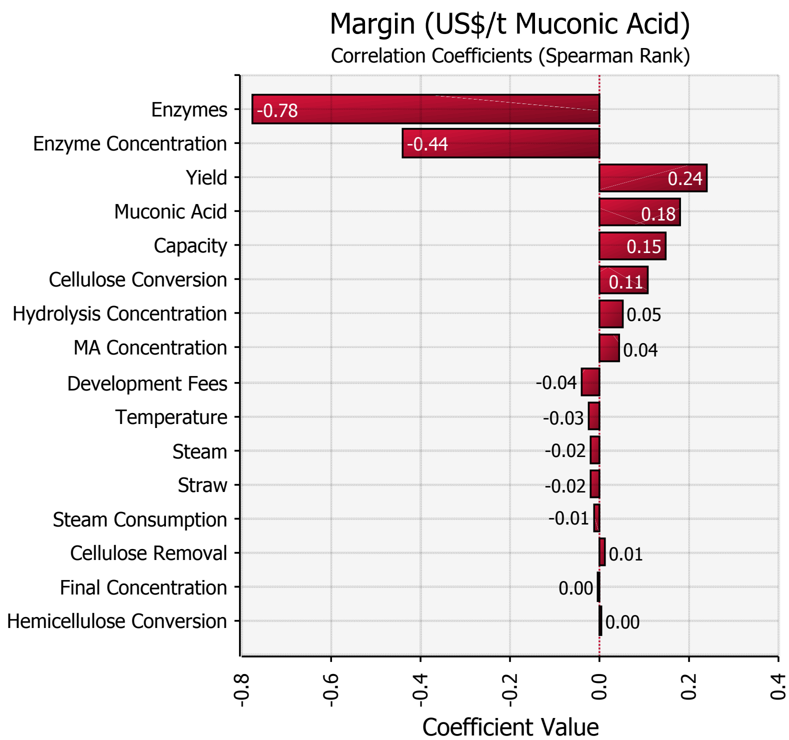


Figure 5.5 Correlation Graph for the Variables Influencing the Product Margin for Muconic Acid Manufacturing

From the graph in Figure 5.5 it is possible to observe that both the enzyme price and the enzyme concentration related to the biomass are the most important variables affecting the margin of the product. Also important are the yield of transformation of sugars to muconic acid, the muconic acid price and the capacity of the plant.

Based on the analysis of the importance of the variables, it becomes clear that a refining of the enzyme price and the enzyme concentration variables is important for a better understanding of the project costs. Besides the highest correlations to the product margin, enzyme cost also makes up to the majority of the variable cost, reinforcing the need to review the variables to which enzyme cost depend. Figure 5.6 displays a pie chart showing the composition of the variable cost, divided in raw materials, utilities and enzyme costs.

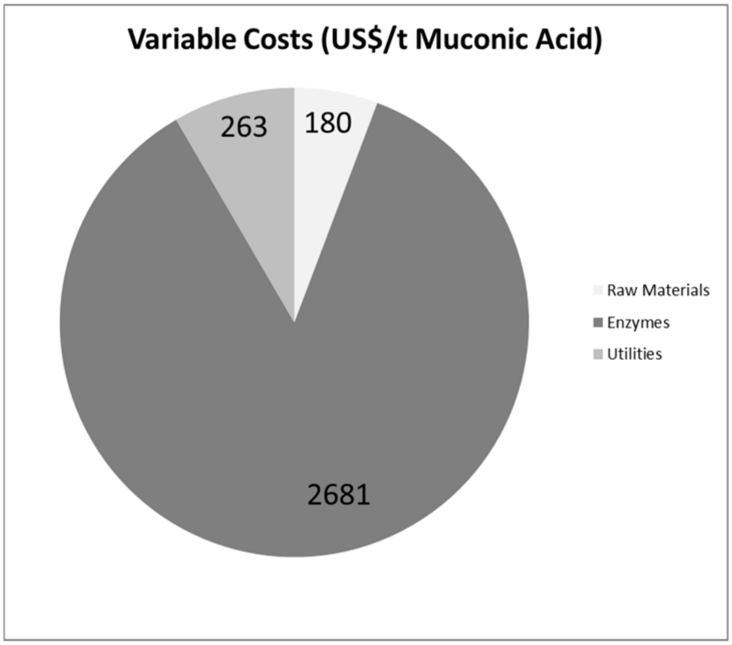


Figure 5.6 Variable Cost Composition for the Muconic Acid Production

Considering the influence of the enzyme costs in the economic results of the muconic acid manufacturing process, it was decided to make a similar consideration for enzyme cost and concentration relative to cellulose as the one taken in the biobutanol case analysis, i.e. enzyme cost varying between US$0.12/kg and US$1.25/kg and enzyme concentration between 4 and 6% relative to cellulose.

The reduction in enzyme cost and consumption caused a drastic reduction in variable cost as expected, and thus changing a lot the economic results of the project. After enzyme cost reduction, a positive margin was possible to achieve and also positive economic results in net present value, EBITDA and internal rate of return. Table 5.7 summarizes the costs and incomes of the muconic acid manufacturing process and Table 5.8 summarizes the economic results obtained by the project to build a muconic acid manufacturing plant.

Table 5.7 Production Costs for Muconic Acid Manufacturing from Biomass after Enzyme Costs Considerations

Costs	
Variable (USS/t Muconic Acid)	657
Fixed (US$/t Muconic Acid)	86
Investment (MUS$)	93
Depreciation (US$/t Muconic Acid)	233
FMC (US$/t Muconic Acid)	976
Raw Materials (US$/t Muconic Acid)	180
Enzymes (US$/t Muconic Acid)	144
Utilities (US$/t Muconic Acid)	263
Margin (US$/t Muconic Acid)	423

Table 5.8 Economic Results for Muconic Acid Manufacturing from Biomass Process after Enzyme Costs Considerations

Economics	
IRR (%)	10%
NPV (MUS$)	24
Capex (MUS$)	93

The internal rate of return is practically the same as the discount rate used in the project, this being the reason for a small, albeit positive, NPV. Although the economic results in this risk analysis revision are not excellent, they give a better perspective on the project development than before, but one should keep in mind that this improvement in results comes with the premise that enzyme prices and consumption are considerably smaller than the ones reported currently in the literature. If the project should continue its development following this analysis, a majority of the resources should be applied to enzyme pricing research and hydrolysis efficiency improvement.

Figure 5.7 displays the product margin distribution for the muconic acid after the considerations to consider narrower enzyme price and enzyme consumption distributions.

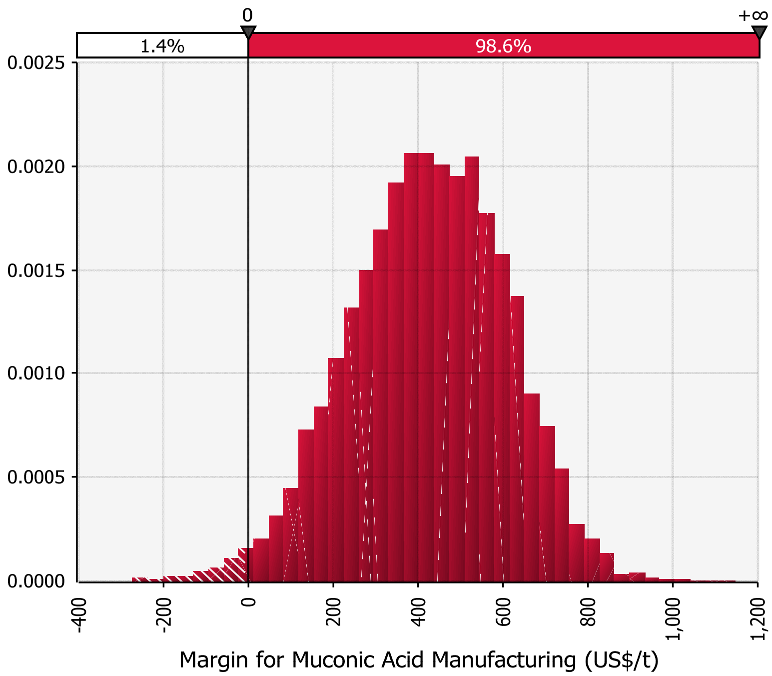


Figure 5.7 Margin for Muconic Acid Manufacturing after Enzyme Cost Considerations

After the considerations to reduce enzyme cost, the probability of achieving a positive margin became closer to 100%, meaning that it would be almost certain that a muconic acid process under these conditions would yield a positive product margin.

Figure 5.8 shows the correlation graph displaying the variables with the highest impact in the margin after the consideration to reduce enzyme costs. As expected, muconic acid price, plant capacity, fermentation yield and solids concentration in hydrolysis became the variables with the highest impact in the margin. Besides enzyme price and hydrolysis efficiency, these should be the other aspects of the project to which most resources should be allocated, market assessment is important to define the muconic acid price and market size, which will define the plant capacity. Technical research would focus on fermentation yields and engineering to increase solids concentration in hydrolysis.

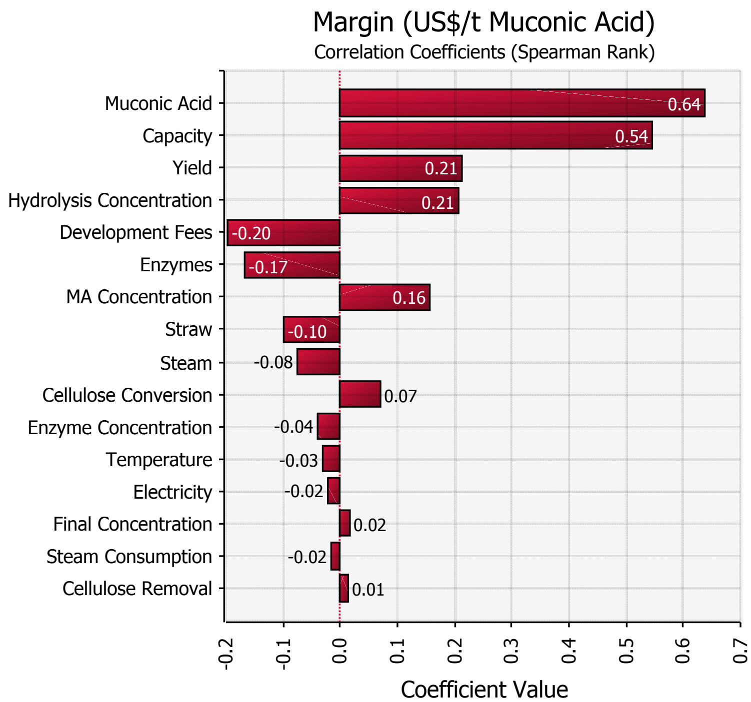


Figure 5.8 Correlation Graph for Muconic Acid Product Margin after Enzyme Cost Considerations

Figure 5.9 shows the distribution of NPV for the muconic acid project with the enzyme cost reduction considerations, an important improvement was achieved since in the original simulation there was a very small probability of the project achieving a positive NPV. In the second Monte Carlo simulation, a close to 75% chance of a positive net present value was achieved.

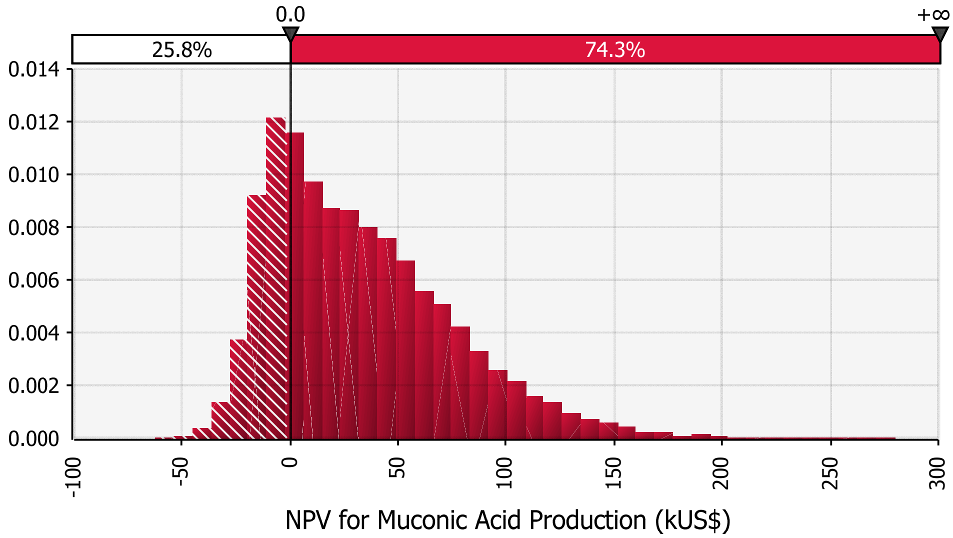


Figure 5.9 NPV Distribution for the Muconic Acid Manufacturing Process

5.5. Risk Analysis Aid in Project Planning

The prospect of a project to produce muconic acid from lignocellulosic sugars is hindered by the high cost of production of the muconic acid and the low market price of adipic acid, the intermediate for which muconic acid should serve as a precursor. It was possible to identify in the economic analysis that the major part of the manufacturing costs were linked to the use of enzyme in biomass hydrolysis, the risk analysis confirms such a prediction. Figure 5.10 shows a tornado graph listing the inputs of the model that are most influential in the net present value of the muconic acid project, the enzyme concentration in hydrolysis and the enzyme costs appear as the two most influential variables, the production capacity of the plant also shows as a relevant influence, reinforcing the need of a thorough market assessment for the production of muconic acid.

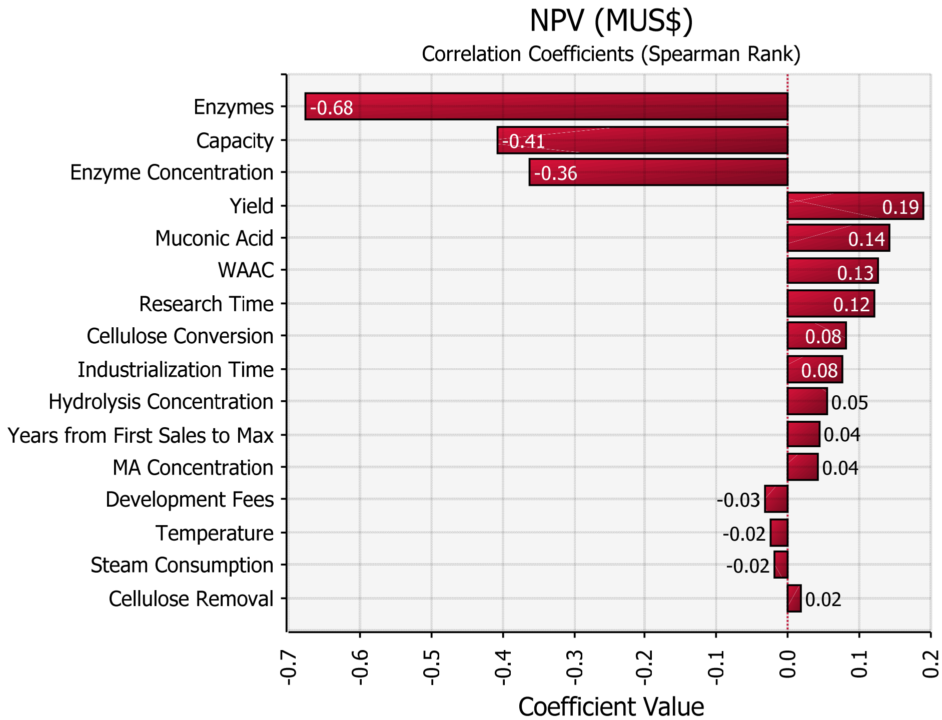


Figure 5.10 Correlation Graph for Internal Rate of Return for the Muconic Acid Plant Project

In a project to produce muconic acid from biomass, the risk analysis conducted according to the methodology here proposed would reveal two main factors as the most important and worth assigning project resources: the market assessment of muconic acid, including research on possible new applications to boost price and volume, enzyme efficiency on biomass hydrolysis and enzyme price for manufacturing cost reduction.

6. CHAPTER 6: COMPETITIVITY OF LIGNOCELLULOSIC SUGARS AS A PRECURSOR FOR BIOPRODUCTS MANUFACTURING

Lignocellulosic sugars have been studied as precursors for production of alternatives to fossil fuels, but the economics of producing fuel from lignocellulosic sugars have proven to be less than ideal. Capital intensive processes and high costs of enzymes yield a high production cost for lignocellulosic sugars, whereas fuels need to be produced at low cost to be feasible, and the fact that fermentation transformation of sugars into known fuels (ethanol and butanol) have low yields contributes to push this scenario further away from feasibility. Reduction of lignocellulosic sugars production prices and de-risking of investments can profit from installation of smaller scale plants that will at first yield even higher production costs due to scale economics but will on the other hand gradually increase scale of production of enzymes and increase technology maturity, which will eventually bring costs down. On this work, economic risk analysis of a hydrolysis process points to the main factors influencing lignocellulosic sugar costs, plant scale is also analyzed and finally a sugar value analysis identifies which markets could be satisfied by lignocellulosic sugars as raw materials. The analysis points that although fuels are harder to reach feasibility with lignocellulosic sugars as raw materials at first, intermediate chemicals, food additives and cosmetics are markets that could be reached out by renewable products produced from lignocellulosic sugars while being profitable at scales necessary to mature hydrolysis technology.

The objective is to investigate the economics of the sugar production from lignocellulosic biomass. A hypothesis of a business dedicated solemnly to producing sugars from lignocellulosic raw material is considered; e.g. a business endeavor that will invest in a plant that produces sugars and then sell it to other plants in which the sugars are transformed into chemicals that could be directed to different markets. An economic risk analysis for the production of lignocellulosic sugars will be carried out along with an assessment of the markets that could be reached by the chemicals produced from these sugars.

6.1. Review of Economics

Work on the economic analysis of the biochemical route have indicated that it is not yet feasible for biofuel production when compared to grain ethanol as well as the thermochemical route biofuel (Wright, et al., 2007) weakening interest in biofuel projects. The main competitiveness factors pointed out are capital investment (Wright, et al., 2007), and feedstock costs (Gnansounou, et al., 2010) (Treasure, et al., 2014) but process costs, especially enzyme costs are also pointed out by some authors (Klein-Marcushamer, et al., 2011) (Albarelli, 2013) Besides economic aspects, other points are mentioned such as public concern with food competition from the crops and technical difficulties in production scale-up (Economist, 2015) (Martins, et al., 2014)

In order to reach economic feasibility, fuels must be produced at high scales and low costs, however other chemical markets could also use lignocellulosic sugars as raw material. Figure 6.1 shows that the processing costs and product value increase in the same direction for both the oil and biomass processing chains. While in the oil chain fuels such as gasoline and diesel are produced in the fractionation column in oil refining, to produce fuels in the biomass chain, it is necessary to crack the biomass into its basic constituents (sugars) and then ferment it into fuels. This poses a problem for biofuel production, since a complex process (enzymatic hydrolysis of biomass, fermentation by microbial strains sometimes requiring special conditions to work, and purification) must be competitive with a more straightforward process (heat fractionation of the oil constituents that form gasoline and diesel). It is possible to infer from such analysis that higher value products such as food additives, intermediates for materials and textiles and higher value solvents should be more promising prospects in terms of competitiveness with the petrochemical chain.

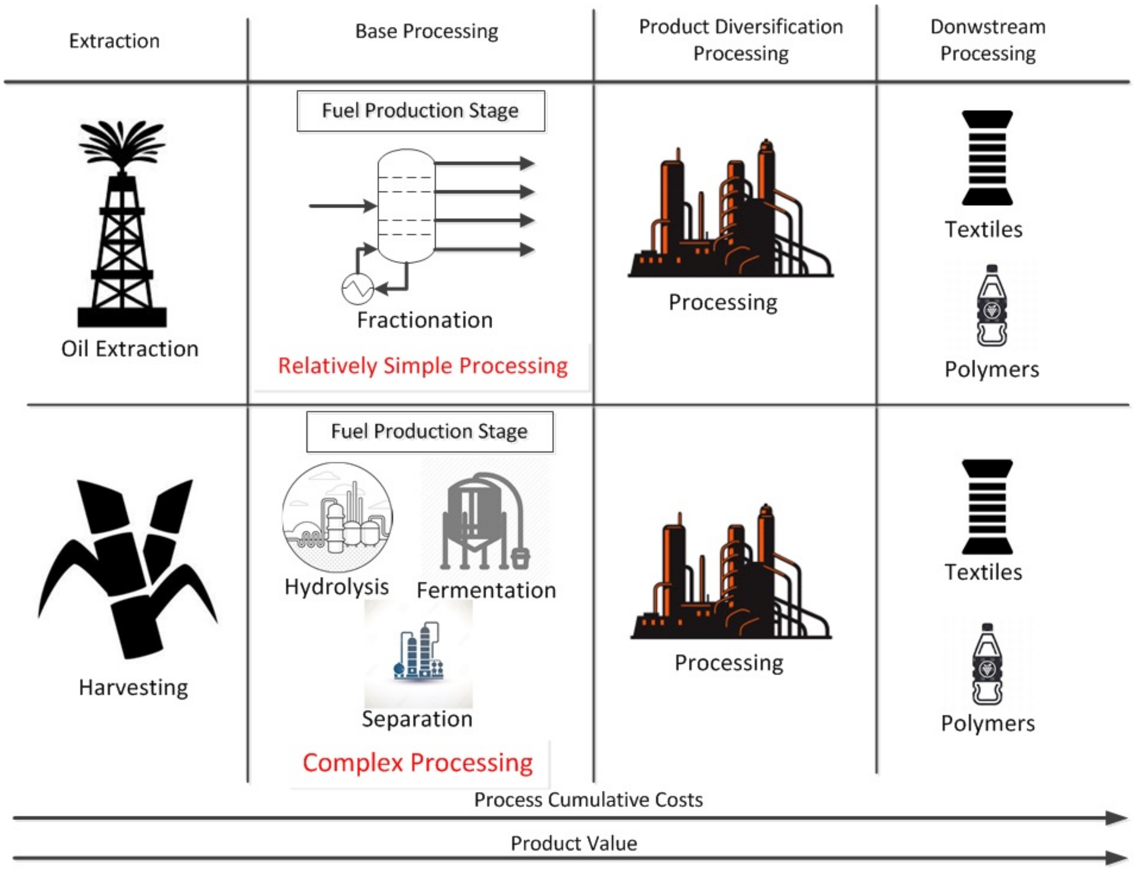


Figure 6.1 Schematic of Value Chain for Oil and Biomass Chains for Manufacturing of Fuel and Chemicals

6.2. Lignocellulosic Sugar Production Process

A method is presented for analysis of lignocellulosic sugars manufacturing technologies; it comprises a mass and energy balance, an economic model, the calculation of the value of the chemical to be produced from the sugar, the risk analysis and finally the decision to be made. Figure 6.2 displays a block diagram with the steps of the methodology, the inputs needed in each step and how they relate to each other.

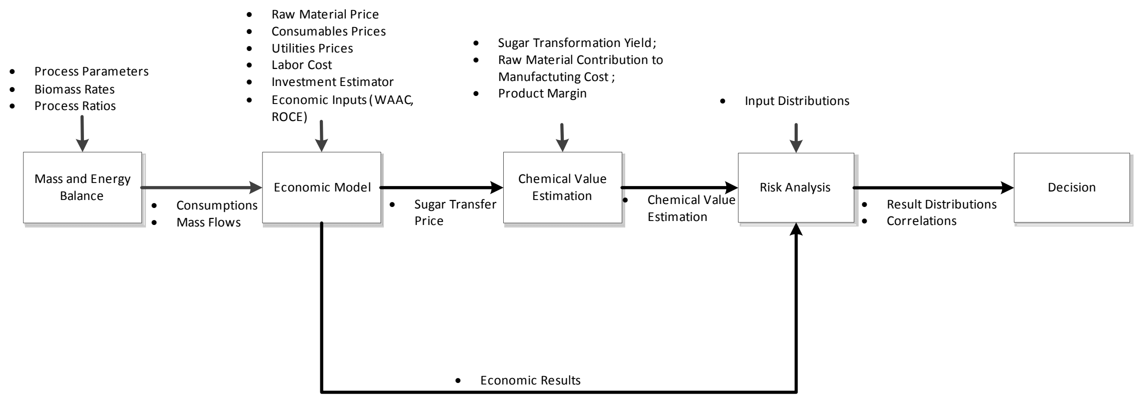


Figure 6.2 Methodology for Biomass Hydrolysis Technology Analysis

Using the work done by Bereche (2011) as the reference base, a mass and energy balance of the process to extract sugars from lignocellulosic material is developed, this tool doesn´t need to be very detailed for a risk analysis to be done, i.e., a mass balance around the main process steps should be sufficient. Figure 6.3 shows the block diagram of the process considered. The mass and energy balance is then used to calculate the specific consumptions of raw materials, consumables and utilities and with this, the variable cost is calculated. As explained in the introduction, the assumption is made that the production of lignocellulosic sugars is an independent endeavor, meaning that all the inputs to the process (biomass, steam, enzyme, water) are considered to be bought at a transfer price. In this configuration no consideration on integration with a first generation mill was done.

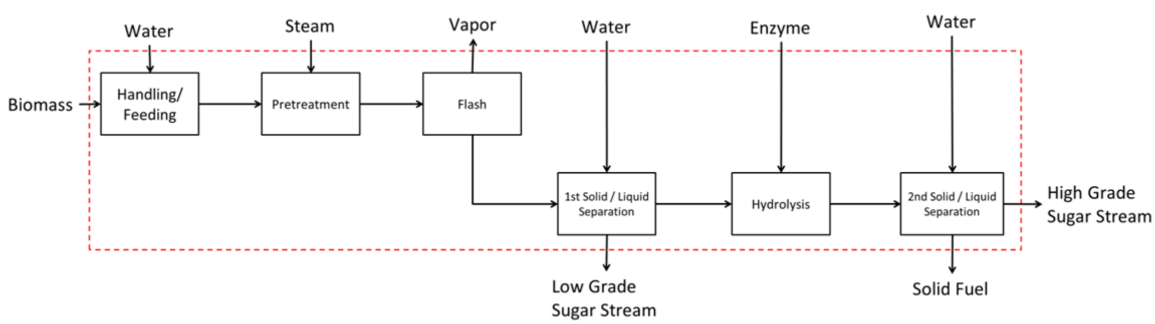


Figure 6.3 Process Diagram for Sugar Production

Biomass enters the process through a feeding system where the biomass is washed and wetted and prepared to be fed at high pressure into the pretreatment vessel. Pretreatment is carried out at 190°C and 12.5bar, the objective is to remove the hemicellulose that is the softer structure of the biomass and increase the exposure of cellulose to enzymatic attack in the following steps. After pretreatment depressurization takes place and water is flashed together with light organic chemicals formed during pretreatment from degradation of hemicellulose such as furfural, low pressure vapor is generated and can be used for biomass pre-heating or considered as credit if used downstream in the sugar transformation process.

After depressurization, the solid matter left is separated from the hemicellulose rich liquid phase through filtration, the hemicellulose dissolved in pretreatment is separated and becomes a byproduct referred to in this work low grade sugar due to the presence of impurities and he fact that the hemicellulose is not completely hydrolyzed into its sugar monomers, xylose. The solid portion comprised of cellulose and lignin proceeds to the enzymatic hydrolysis tanks where enzymes break the cellulose polymer into its glucose monomers, hydrolysis temperature is low, around 50°C and residence time is very large, 72h.

Fixed costs were calculated in the same way as in the biobutanol and muconic acid cases, explained in sections 2.3.2 and 4.2.3.1, investment for the sugar manufacturing plant was estimated using the process step score method also in the manner as for the biobutanol and muconic acid cases, as explained in section 2.3.1.2. Risk analysis was run according to the exposed in the section 3.4 and done in the Chapters 4 and 5.

6.3. Economic and Risk Analysis of Lignocellulosic Sugar Production

In Table 6.1 the inputs for the model are listed with its main values, range and distribution types.

Table 6.1 Inputs and Distributions for Economic and Risk Analysis.

Main Variables in Risk Analysis	Probable Value	Máximum	Minimum	Distribution
Prices				
Biomass (US$/dry t)	35	48	21	Normal
Enzyme (US$/kg)	10.2	10.5	0.15	Triangular
Steam (US$/t)	12	40	8	Triangular
Electrcicity (US$/MWh)	71	42	100	Normal
Economic Premises				
Plant Throughput (t/h of dry biomass)	50	80	20	Discrete
WAAC (%)	9.9	13.2	8.1	Triangular
Price Ratio Between High Grade C6 and Low Grade C5 (%)	10	50	25	Triangular
R&D Costs (kUS$)		3000	1200	Uniform
R&D Time (years)	3	5	3	Discrete
Industriilzation Time (years)	2	4	2	Discrete
Sales Ramp-up (years)	2	4	2	Discrete
Capex Innacuracy Multiplier		0.6	1.5	Uniform
Process Parameters				
Steam Consumption in Pretreatment (t/t wet biomass)	0.55	0.76	0.34	Uniform
Hemicellulose Removal (%)	61	86	38	Uniform
Cellulose Conversion to Hexoses in Hydrolysis (%)	69	96	40	Uniform
Hemicellulose Conversion to Pentoses in Hydrolysis (%)	46	64	27	Uniform
Hydrolysis Solids Concentration (%)	10	20	7	Triangular
Enzyme Consumption (% over cellulose)	11	12	4	Triangular
Conversion Yield from Sugar to Chemical		0.95	0.27	Uniform
Contribution of Raw Material Cost in Full Manufactuting Costs (%)		70	30	Uniform
Chemicals Margin (%)	15	60	0	Triangular

The manufacturing cost calculations show that enzyme is the greatest impact on sugar manufacturing costs. Figure 6.4 shows the cost breakdown of lignocellulosic sugars for two enzyme prices, the higher price found by Klein-Marcushamer (2011) and a lower value based on soy protein. For a plant that processes 50 dry tons of biomass per hour and investment of around 60 MUS$ was estimated.

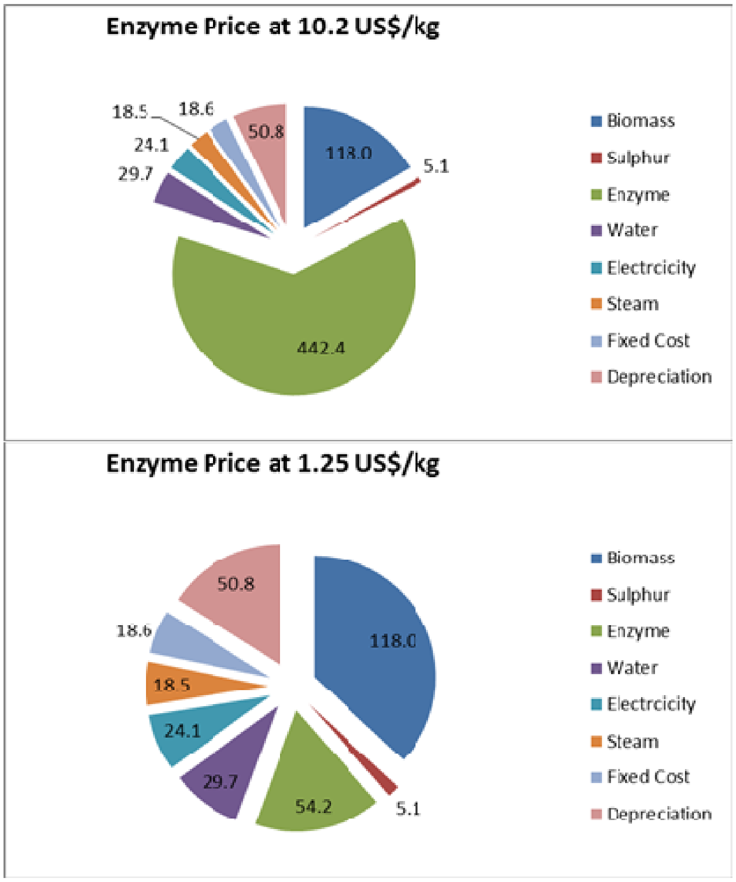


Figure 6.4 Cost Breakdown for high a and a low enzyme price (in US$/t)

Even in the lower price case the weight of enzyme in the manufacturing cost is considerable, lower only than raw material and slightly higher than the investment. A Risk analysis run with the distributions proposed in Table 6.1 showed a strong correlation between the sugar transfer price calculated with enzyme price. Figure **6.5** shows the influence of enzyme price and consumption in the calculated sugar transfer price and the distribution obtained.

The sugar transfer price was calculated using Eq 2.

$$TP = FMC + \frac{Capex * ROCE}{Production} \qquad \text{Eq 2}$$

Where:

TP: Transfer Price of the lignocellulosic sugars ($/t);

FMC: Full Manufacturing Costs of the lignocellulosic sugars ($/t);

Capex: Capital invested in the plant ($);

ROCE: Return over capital Employed (%);

Production: Product Volume of in a year (t/y);

The transfer price of sugar was limited by a higher and lower limit defined by the historical prices of sucrose sugar in Brazil, data for sugar prices were obtained with the Center for Advanced Studies in Applied Economy (CEPEA, 2015) the higher limit was set at the 75% higher price registered in the last 10 years at US$354/t and the lower limit was defined at 70% of the lowest price registered at 76US$/t.

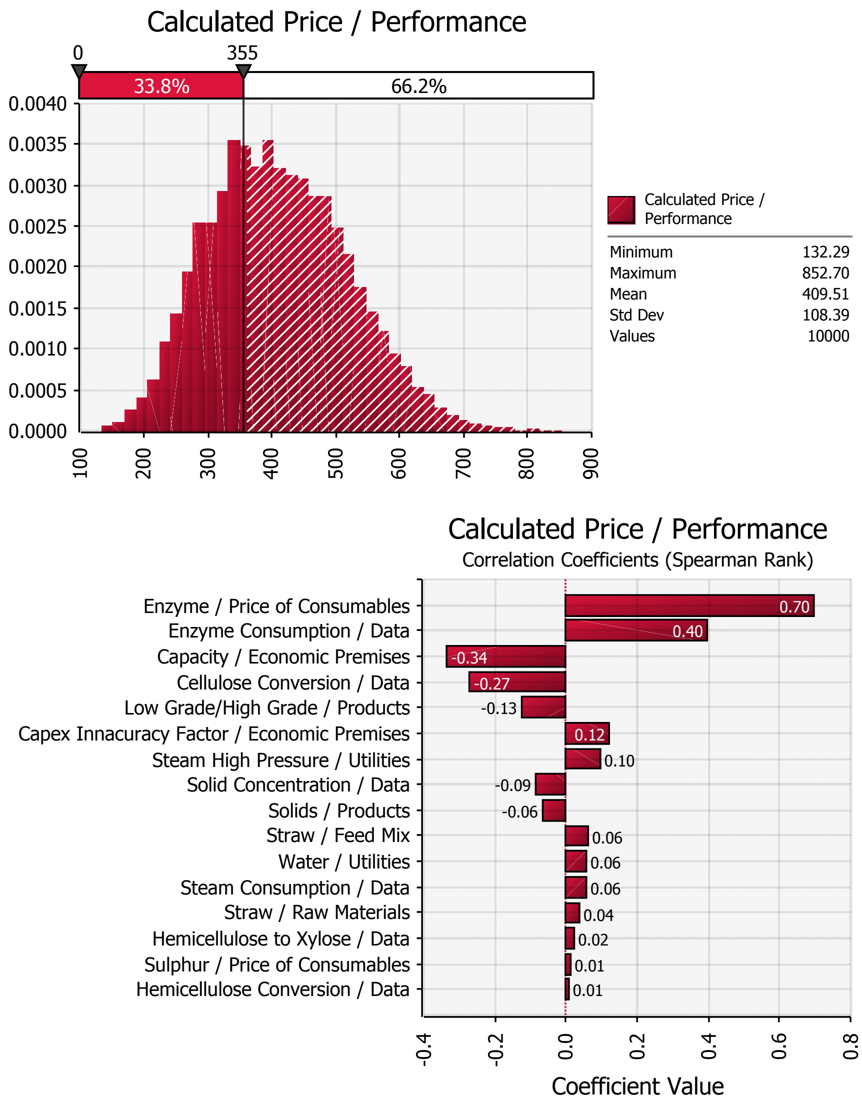


Figure 6.5 Inputs with higher correlations to the calculated sugar transfer price (bottom) and the distribution of the calculated sugar transfer price (top) for the Risk Analysis Run 1.

The correlations between the inputs and the sugar transfer price show the high impact of enzyme cost and consumption in the sugar value. The wide range found in the literature for the enzyme price contributes to this conclusion. It is possible to evaluate in the sugar price distribution that the probability of the sugar price being higher than the sugar price high limit determined is 66%, meaning that there is a 66% chance that the business would have to sell the sugars produced for a lower price than the necessary to obtain a return over capital employed (ROCE) of 25%. A sensitivity analysis of the enzyme price over the main economic metrics such as net present (NPV) value, product margin and earnings before tax depreciation and amortization showed the importance of the enzyme price and pointed to the conclusion that in to reach economic feasibility, the enzyme prices should be lower than US$5000/t (Figure 6.6).

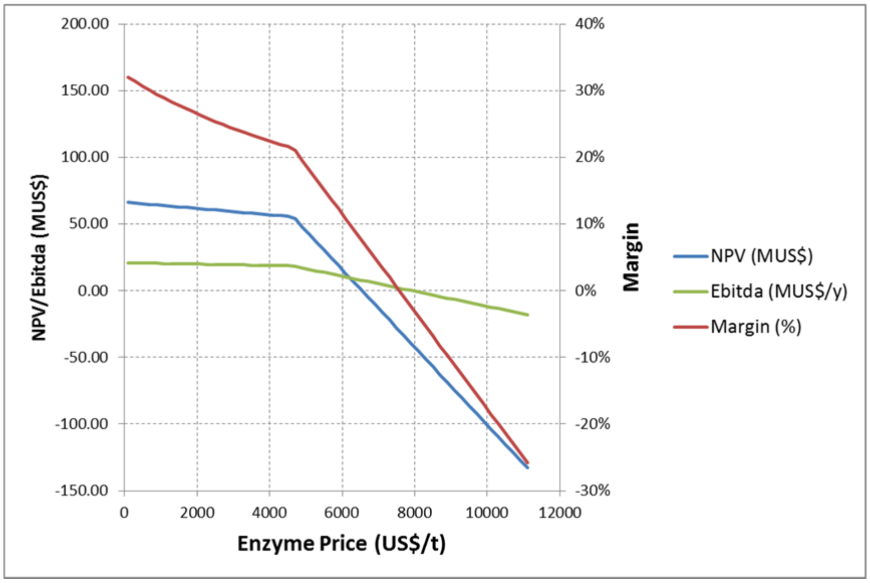


Figure 6.6 Evolution of NPV, Ebitda and Margin with enzyme price

The difference in the inflexion of the three curves with enzyme prices higher than US$5000/t is due to the fact that after such value, the calculated transfer price of sugar is limited by the maximum price allowed in comparison to the sucrose price in Brazil as shown in Figure 6.7.

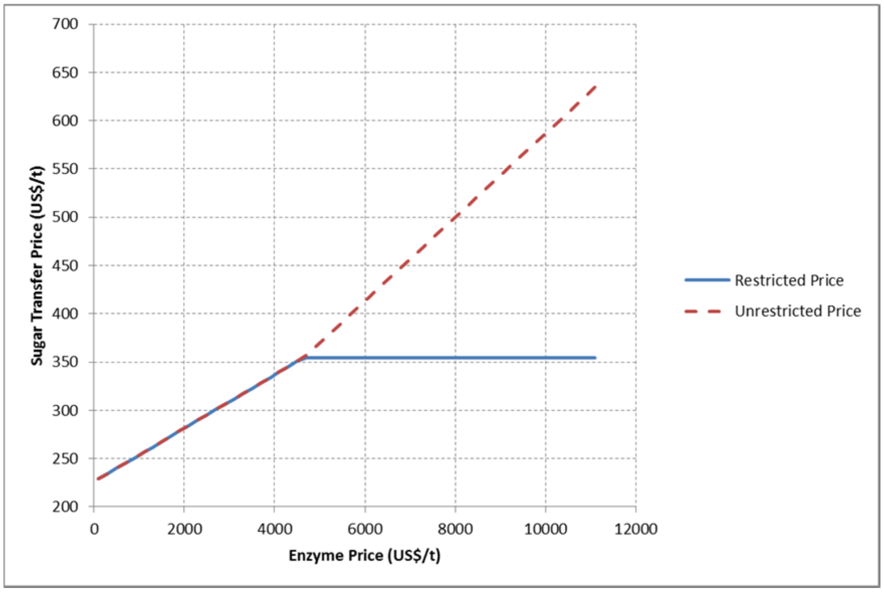


Figure 6.7 Restricted and unrestricted transfer price evolution with enzyme price

Based on these results and mainly in the fact that the sugar transfer price would often result in a higher value than the higher limit set, it was decided to run a second risk analysis using a new enzyme price distribution (Figure 6.8). The distribution of enzyme price in the second risk analysis run has a smaller range than the first run, so the sheer range of the variable will no longer play a role on its high correlation to the economic results. Also, with advancements in enzyme production and negotiations between enzyme producers and biorefineries, it is probable that enzyme price will fall into the smaller range showed in Figure 6.8. A more detailed discussion on enzyme price and consumption can be found on sections 4.2.1.5 and 4.2.3.1.

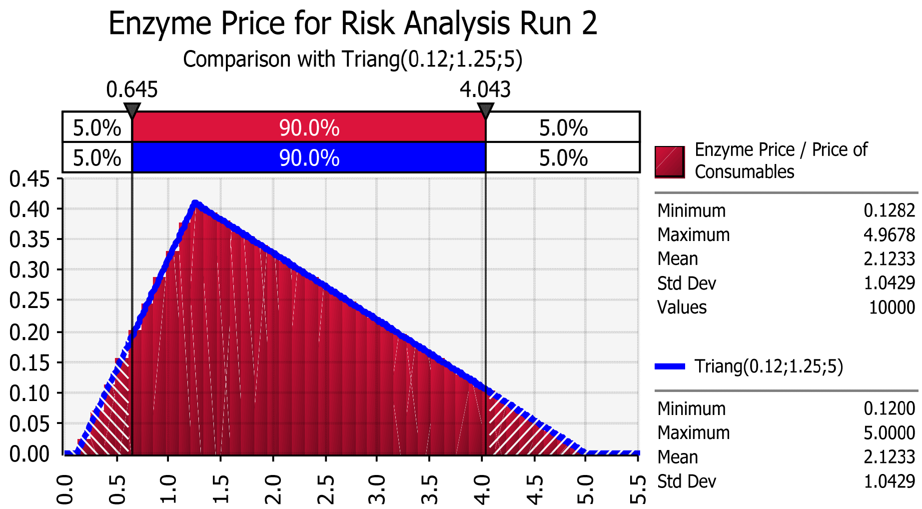


Figure 6.8 Enzyme price distribution for Risk Analysis Run 2

The second risk analysis run, nominated Run 2 presented a probability of the calculated sugar transfer price being higher than the established limit of US$364.7/t of 40% versus 66% in Run 1, meaning that in the case of enzyme price being lower than US$5/kg, the probability of the sugar manufacturing business having to sell sugars at prices lower than the ideal, is 40%. The correlations between the inputs and the sugar calculated price also change with the smaller enzyme price range, but still it has the second highest correlation. The highest correlation is the capacity of the plant, also, biomass transformation yield and the inaccuracy of capital investment present important correlations. Such high correlations to these inputs lead to the conclusion that the aspects of the project to which resources should be allocated are raw material, hydrolysis yield, investment and enzymatic hydrolysis. Figure 6.9 shows the sugar calculated transfer price distribution and the correlations of the inputs to the sugar value, the correlation graph should be interpreted as follows: the size of the bars indicate the importance of the correlation; the bigger the bar, the bigger the correlation. The bar direction indicates if the input is directly or inversely proportional to the result, for example, the bar representing capacity is directed to the left, meaning that capacity and sugar transfer price are inversely proportional, the higher the capacity, the smaller will be the sugar transfer price . The bar representing enzyme price is directed to the right, meaning that enzyme price and sugar transfer price are directly proportional, the higher the enzyme price, the higher will be the sugar transfer price.

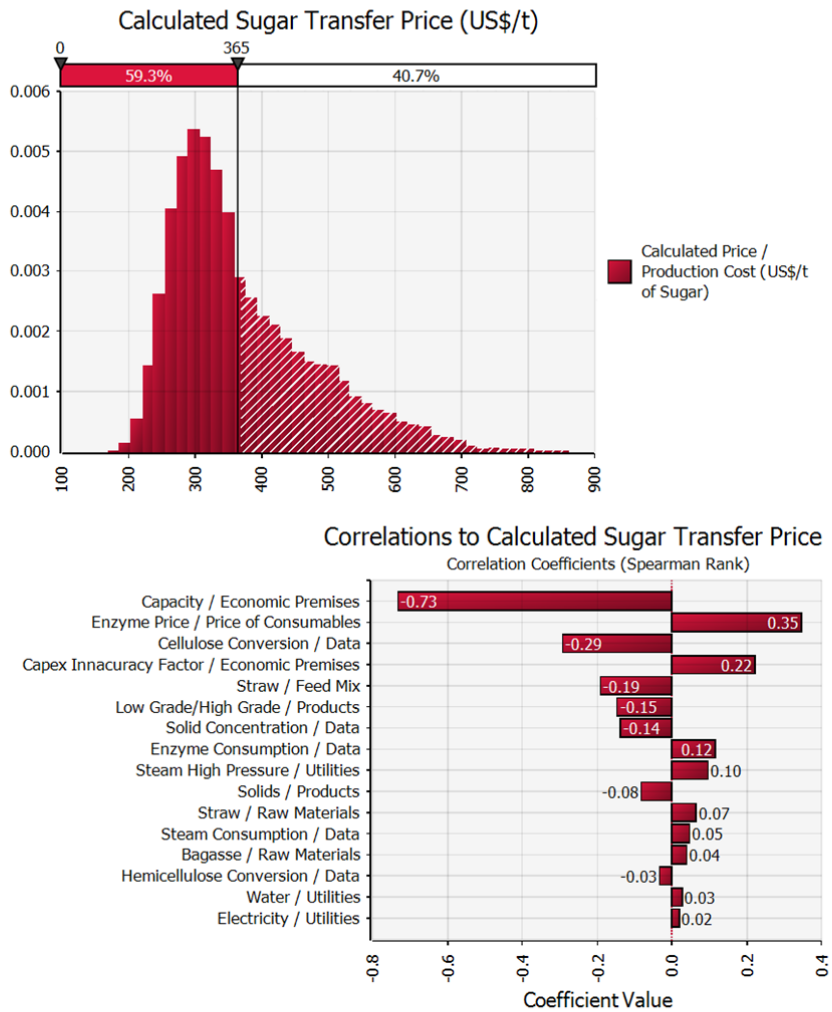


Figure 6.9 Inputs with higher correlations to the calculated sugar transfer price (left) and the distribution of the calculated sugar transfer price (right) for the Risk Analysis Run 2.

It is important to note in this example how a wider distribution can affect more the correlations in a Monte Carlo simulation, for this reason, care should be exercised when assigning distributions to the inputs. In the case of the enzyme price, a wide range of values can be found in the literature so it is advisable when analyzing a hydrolysis process to try different distributions, wider and shorter, to understand better the dynamics of this input.

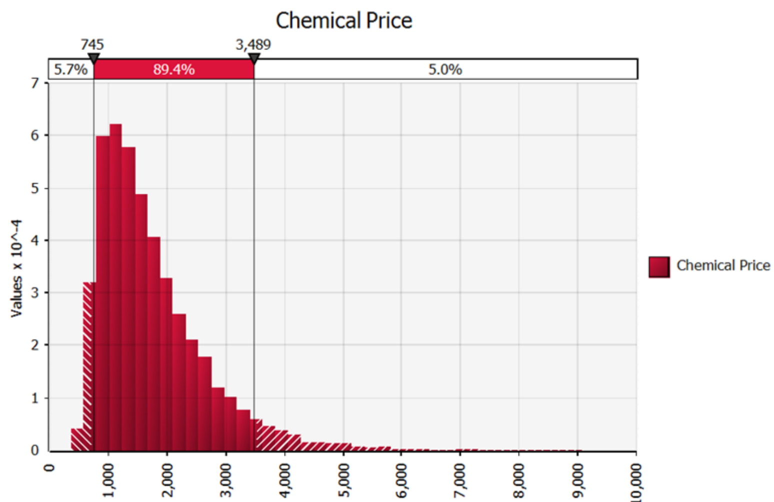
The sugar transfer price of the risk analysis Run 2 was used to estimate the downstream chemical value according to Eq 3.

$$\mathrm{ChPrice} = \frac{\mathrm{TP}}{\mathrm{TY} * \mathrm{RMC} * \mathrm{Margin}} \qquad \text{Eq 3}$$

Where:

- ChPrice: Downstream chemical price ($/t);
- TP: Transfer Price of the lignocellulosic sugar ($/t);
- TY: Transformation yield of the downstream process (%);
- RMC: Raw material cost contribution to the chemical manufacturing cost (%);
- Margin: Product sales margin applied by the downstream chemical producer (%);

This analysis generally intends to predict the distribution of values of a chemical produced via lignocellulosic sugars as raw material, and then, by looking into the distribution, try to predict to which market the lignocellulosic sugars should be directed. Petrobras (the Brazilian state oil company), states that price of gasoline in Brazil, before taxes and distribution costs should be around US$750/t (Petrobras, 2015), this is the value to which we should compare the calculated chemical value to estipulate the competitiveness in the fuel market. Figure 6.10 shows the distribution of the calculated downstream chemical price, the value of US$750/t was marked on the graph to calculate the probability of a chemical value competitive with fuel being achieved.



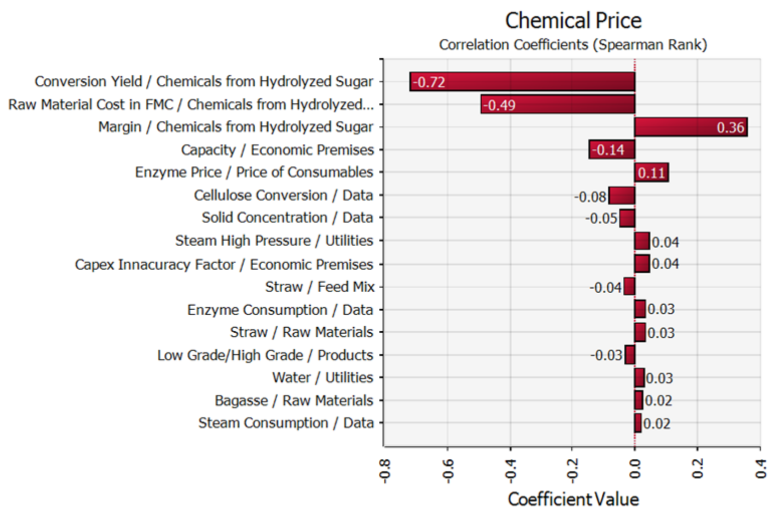


Figure 6.10 Downstream chemical value estimation for high grade cellulose sugars as raw material.

The probability that the downstream chemical produced from lignocellulosic sugars would be competitive with fuel is 5.7%, and there is a probability of 5% that the chemical value would overcome US$3500/t, suggesting that the chemical produced from high grade cellulosic sugars would certainly be competitive in markets at that price level. It is possible also to observe from Figure 6.10 that the highest correlations to the chemical price are in the following (decreasing) order: the yield of transformation, the weight of raw material cost in the full manufacturing cost and margin.

It is in the business developer interest to analyze the chemical value in light of the higher correlation: the yield of transformation of the sugar, Figure 6.11 shows the cloud of results of the chemical value and a tendency line indicating the most probable value to be expected at a given sugar transformation yield. It is possible to see from the tendency line that if the downstream process presents a high yield of transformation, chemical value decreases, and its distribution becomes narrower (right arrow), therefore becoming more competitive, if the downstream process presents a low yield of transformation, the value increases, and, the distribution becomes wider (left arrow), decreasing competitiveness of such a chemical. The reason for the wider distribution is that the lower the yield, the higher the raw material cost to the chemical, and the subsequent factors of raw material cost contribution and margin will be applied to higher values. It is sensible to expect that this result would represent real processes, since lower yields would probably mean higher energy and investment costs for separation of impurities.

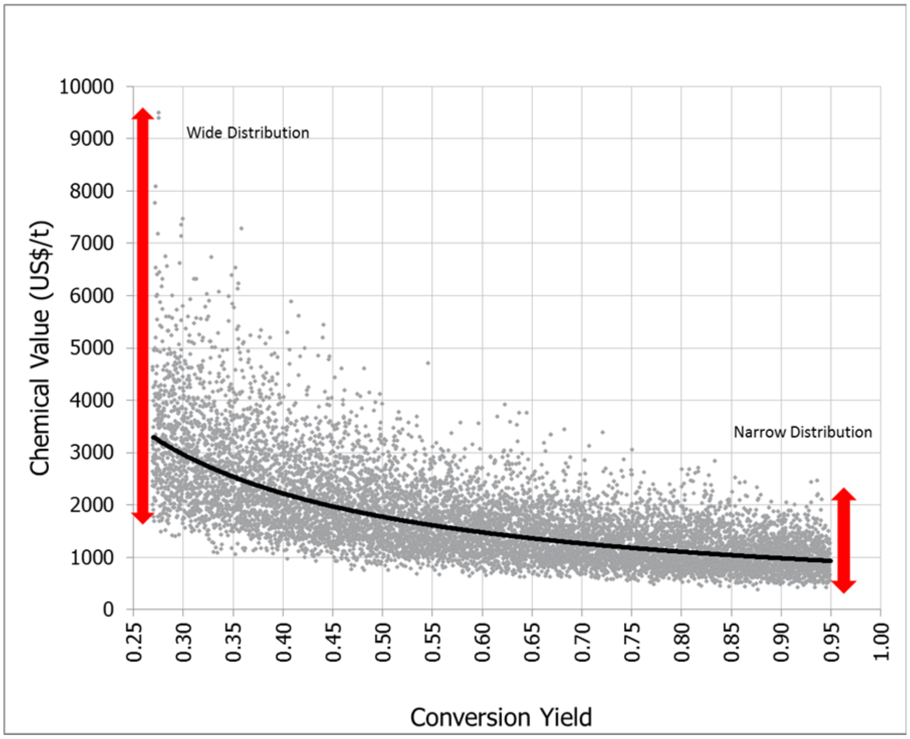


Figure 6.11 Result cloud and tendency line for chemical value versus sugar conversion yield.

The results of chemical value were separated in two different levels regarding the margin of the chemical. A lower margin of 15% was considered to typically represent a generic commodity chemical and a higher margin of 60% was considered to represent a generic specialty chemical. Figure 6.12 shows that the two distributions overlap for the most part, meaning that over 50% of the specialty chemicals are in the same range as 90% of the commodity values, however, the specialty distribution is wider, meaning that a specialty chemical would be competitive or not depending on the other two calculation parameters: the transformation yield and the raw material contribution to full manufacturing cost.

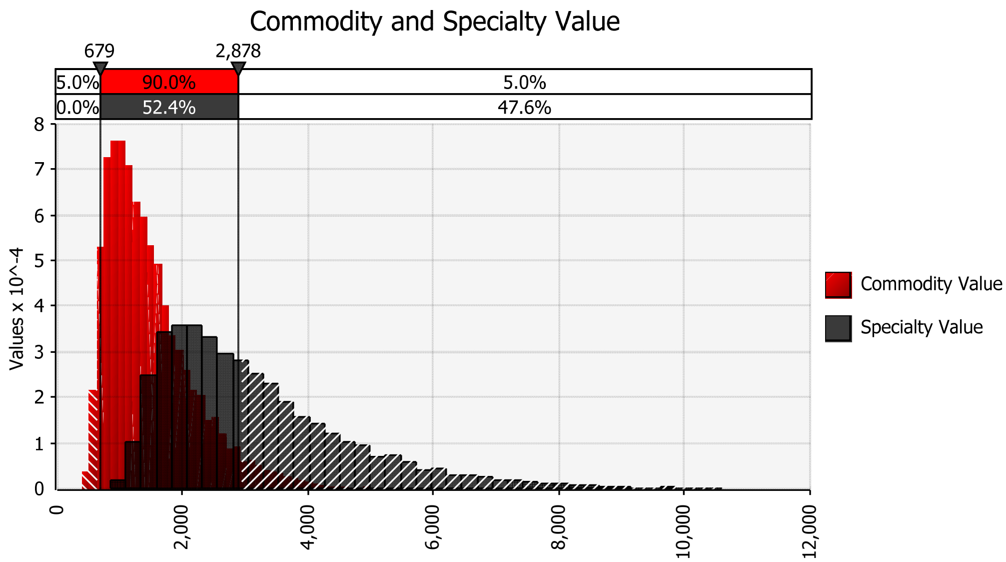


Figure 6.12 Chemical value distribution for two levels of applied margin: 15% representing commodity chemicals and 60% representing specialty chemicals

When the most probable value line is observed separately for the two distributions versus the yield of transformation of sugars, the difference in the chemical value between the two alternatives becomes clear. Figure 6.13 is similar to Figure 6.11 since it also represents the cloud of resulting chemical values, differing only that the actual cloud points were suppressed so the tendency lines could be better observed.

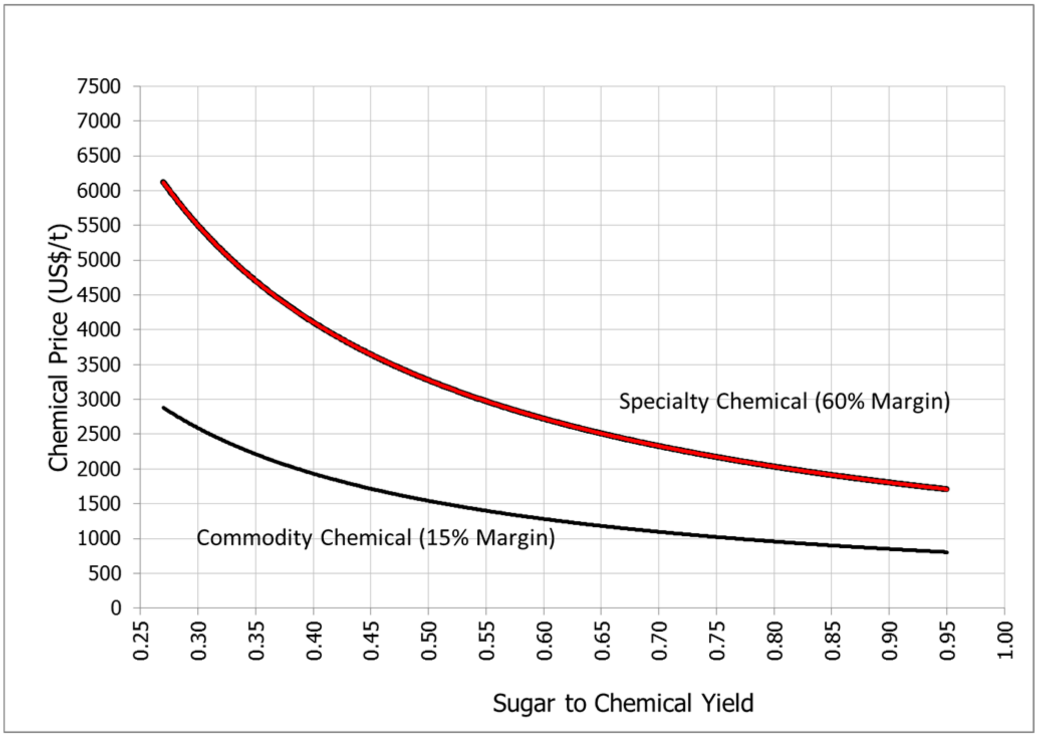


Figure 6.13 Specialty and commodity chemical values versus sugar transformation yield (tendency line)

Producing chemicals from the high grade cellulose sugars could reach markets that offer higher value for product than fuels. If the commodities market is considered, for a process with a low yield of transformation, i.e., fermentation, chemicals with market value between US$1500/t and US$3000/t should be targeted, while in process with higher transformation yields, such as esterification or hydrogenation, markets with prices under US$1000/t could be achieved. The same analysis would apply for specialty chemicals: low yield processes would result in chemicals valued above US$4000/t whereas high yield processes would result in specialty chemicals valued in the range US$1500/t - US$2000/t, with improved competitiveness.

As shown in Figure 6.3 a low grade sugar is also produced in the process from the hemicellulose removed in the pretreatment, the value of this low grade sugar was estimated as a percentage varying from 10 to 50% of the high grade cellulose sugar as mentioned in Table 6.1. Using the same method as for the high grade sugars, the downstream chemical value using the low grade hemicellulose sugar as raw material was estimated along with a value distribution. Figure 6.14 shows the distribution of the downstream chemical value calculated.

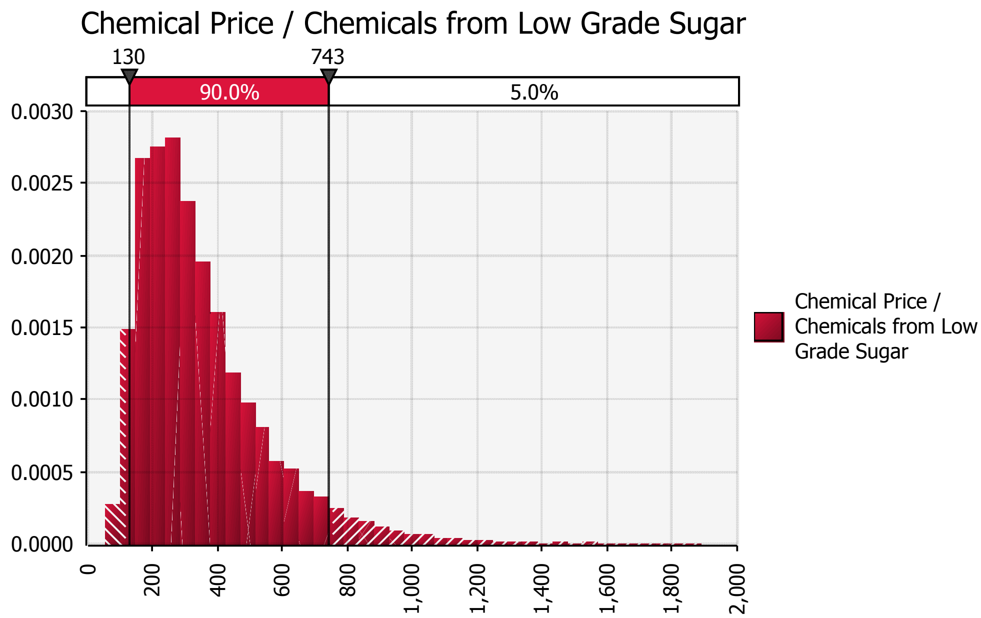


Figure 6.14 Downstream chemical value estimation for low grade hemicellulose sugars as raw material.

Chemicals produced from the low grade sugars from hemicellulose are competitive with fuel prices, suggesting an opportunity for the introduction of biofuels in the market. Since value for low grade sugars are calculated as a percentage of the high grade sugar, it is possible to conclude that such an opportunity would appear depending on the existence of a market for higher value chemicals produced from the high grade sugars via enzymatic hydrolysis.

6.4. Using the Risk Analysis for the Development of the Technology

The risk analysis performed on the technology for the transformation of biomass into lignocellulosic sugars indicated that the variables relating to the enzyme cost in the process had the highest correlation to the economic results of the technology. Researchers looking into developing such technology will have to put an important amount of resources into investigating how to lower enzyme prices and how to raise process efficiency in using them (enzyme concentration, enzyme recycle, etc.). Yield of the cellulose conversion into sugars also has an important correlation to the cost of producing the lignocellulosic sugars, meaning that it is a pivotal process result to improve.

Also, the risk analysis showed that raw material prices and plant capacity are very influential on the sugars cost of production, ranking even higher than Capex variations. This proves that business development is an effort as important as technical development in making lignocellulosic sugars economically feasible, finding a raw material source at competitive cost and increasing the plant capacity by aggregating as many downstream processes as possible can be the factor that turn lignocellulosic sugars feasible for renewable chemicals and fuels.

7. CHAPTER 7: CONCLUSIONS

7.1. Base case I: Biobutanol;

For the case of the biobutanol production, it was possible to apply stochastic economic and risk analysis to the project of a biorefinery integration between an existing sugarcane mill and a new biobutanol facility. Two scenarios were evaluated:

- Scenario A, integrating a 80kt/y biobutanol facility into a mill with a sugarcane crushing capacity around 9 million tons of sugarcane per year, and
- Scenario B, integrating a biobutanol facility with a production capacity around 30kt/y with a sugarcane mill with capacity of 3.5 million tons per year of sugarcane crushing capacity.

The economic figures of the project were analyzed from two different points of view:

- The biobutanol plant as an isolated venture, buying biomass and utilities from the mill and
- The integration of the biobutanol plant with a sugarcane mill to from a biorefinery.

In Scenario A, the risk analysis identified a probability of 34% of the project achieving a positive NPV at a discount rate of 11%. In all cases and scenarios, NPV for the project of the integration of the biobutanol plant into a sugar and ethanol mill were better than the NPV for the isolated biobutanol plant. For Scenario A, the probability of an above zero NPV for the integration project was found as 66%.

The variables that presented the higher correlations to the NPV of the project were:

- Enzyme price and enzyme consumption;
- Butanol price;
- Investment Cost accuracy;
- Solids concentration in the hydrolysis.

Enzyme price and enzyme concentration variables were modified for a second Monte Carlo simulation run based on the literature that presents a wide range of values for enzyme price and consumption, price ranging from 10 to 0.1 US$/kg and consumption ranging from 10% to 4% over cellulose hydrolyzed. An optimistic approach to the values of enzyme price and consumption was taken.

After the second Monte Carlo simulation run, the probability of the biobutanol project to achieve a positive net present value increased from 34% to 65%, the probability of the integration project achieving a positive NPV increased from 66% to 91%.

Scenario B consisted of a lower capacity biobutanol plant and mill, as expected the economic results achieved for this scenario were worse than for scenario A. For the biobutanol project, the probability of achieving a positive net present value is 4.7% and for the integration project 22%. In the same way as in scenario A, the variables with highest correlation to the NPV were identified and again, enzyme price and consumption were refined for a second Monte Carlo run. In the second run, the probability of the biobutanol project achieving a positive net present value increased from 4.7% to 25% and for the integration project the increase was from 22% to 57%.

Table 7.1 summarizes the results obtained in the risk analysis of the biobutanol case

Table 7.1 Summary of the Biobutanol Risk Analysis

Scenario	Description	Run	Biobutanol Plant	
			isolated	integrated
A	9M ton/y of sugarcane crushed, 80 kt/y of biobutanol produced	1st	34% of + NPV	66% of + NPV
		2nd	65% of + NPV	91% of + NPV
B	3.5M ton/y of sugarcane crushed, 30.1 kt/y of biobutanol produced	1st	4.7% of + NPV	22% of + NPV
		2nd	25% of + NPV	57% of + NPV

Both scenarios showed that a biorefinery project consisting of a biobutanol plant integrated into a sugarcane mill would have a moderately good chance of being a profitable project as long as enzyme price and consumption are improved from the current levels. Also, the fact that the integration economic results were better than the economic results for the biobutanol plant isolated points to the fact that the prices of the biomass and utilities being sold to the biobutanol plant from the mill are important for the economic success of the endeavor if the owner of the mill and the owner of the biobutanol plant are different investors.

A last exercise done on the biobutanol case was to execute a risk analysis on the same process but using less information as input. The results were more optimistic for the probability of the NPV being greater than zero than the previous analysis, which shows an important aspect of the methodology, it is desirable that the it will yield a more optimistic result for an earlier and less detailed analysis as this prevents the stopping of a project due to an excessively pessimistic early stage evaluation. Also, the correlations found between the inputs and NPV were generally the same as the previous analysis, such as enzyme price, enzyme consumption and solid concentration, with the difference that process yields had higher correlations with NPV than in the previous analysis.

The methodology yielded results that are consistent with different levels of detail in the project and demonstrated its usability as a tool to aid project development.

7.2. Base case II: Muconic Acid;

In the muconic acid case it was possible to employ the methodology proposed in this work in a project with low level of information opposed to the biobutanol case, where a good deal of information was available since the ABE fermentation is a well-studied technology.

Economic results for the muconic acid plant project became limited by the high production costs and the low product price, since muconic acid was defined as a precursor to adipic acid, limiting its market price. The first economic analysis resulted in a full manufacturing cost (FMC) higher than the price of the product, indicating the unfeasibility of the project. The risk analysis indicated there a chance of approximately 8% that the margin of this process would positive, that is, the chance that the value of the products and byproducts would surpass the manufacturing costs.

The enzyme costs, yield of transformation, muconic acid price and plant capacity were identified as the variables with the highest impact in the product margin, and similarly to the biobutanol case, enzyme price and consumption were redefined to more optimistic estimates for the running of a second Monte Carlo. In this second run, the probability of the product margin being positive was near to 100%, indicating that in the scenario of lower enzyme price and lower consumption the muconic acid process could be economically feasible. In such conditions, the probability of the project achieving a positive net present value is near 75%.

The risk analysis indicated that for a project for producing muconic acid from biomass, the enzyme price and the enzyme consumption are key factors. Additionally, resources should be allocated to improving the fermentation yield and to develop a market analysis to better identify the muconic acid market price and demand that would determine the adequate plant capacity.

7.3. Lignocellulosic Sugars Competitiveness;

Risk analysis of the lignocellulosic sugars production indicated that the process parameters featuring the highest impact on the lignocellulosic sugar transfer price are the enzyme cost, capital investment and raw material cost. It is important, then, that research and development efforts are directed to mitigate these risks.

The distribution of the value of the downstream chemical produced from hydrolyzed cellulose sugars showed a 5% chance that such value would be higher than US$3500/t and 5.7% chance the value would be lower than US$750/t, meaning that it would have a very low probability of being competitive with fossil fuels. However, at higher value markets that could pay over US$3500/t, it would almost certainly be competitive. Besides that, the higher value for hydrolyzed cellulose sugars would allow the lower grade hemicellulose sugar extracted in the pretreatment to be sold at a lower price, resulting in downstream products probably competitive with fossil fuels, since its value distribution resulted with 90% confidence in a range between US$130/t and US$750/t.

These results point to the direction of a development that would prioritize the more expensive production of sugars from cellulose to the production of chemicals with high added value, while developing the lower cost sugars from hemicellulose to become available for biofuel development.

7.4. General conclusions;

The cases studied in this work demonstrated that the use of stochastic methods can improve the analysis of processes and projects. The economic risk analysis method proposed using Monte Carlo simulations (a stochastic method) allowed analyzing the projects at a level that would not be possible with an economic analysis using solely deterministic methods. In all cases, an initial economic analysis using deterministic methods yielded results that would lead to the termination of the projects due to low economic attractiveness and in all cases, risk analysis was successful in identifying the variables of the process that contributed the most to the results, indicating the leverages of the project where to focus the activities. After the refinement of the variables that affected the most the economic results, the probability of the projects achieving the desired economic results, i.e., positive NPV improved considerably, indicating that there is a chance that these projects would yield attractive results if the variables with higher impact in the project were further studied and optimized, for example, price of the enzyme and consumption of the enzyme.

The risk analysis for the different cases have shown that enzyme price and enzyme consumption, due to the high variability presented in the literature, are the main variables affecting feasibility of projects that intend to produce chemicals from biomass by using enzymatic hydrolysis. The lack of an accurate definition on these variables can lead to wrong decisions in these projects. Further work is needed for a prediction of what the enzyme price would be when biomass hydrolysis plants come online.

The importance of the market analysis in such projects was also shown in this work, in all risk analysis, because product price and plant capacity are highly correlated to the economic results. In early stage analysis such as those demonstrated in this work, market analysis is usually not available, but the results show the importance that an effort in the definition of market prices and volumes should be put forth right the beginning of the project.

The accuracy of the capital investment estimation also presented high impact on the economic results. Usually, in early stage analysis, there is no available data on equipment and installation costs for precise capital investment estimation; in many cases not even an order of magnitude type of estimation is possible due to lack of process and design information. In spite of the scarcity of data, there are a few alternatives to estimate the plant investment in early stage analysis, for example by using the cost of similar plants or by using estimation methods based on a small amount of process information. In this work the Process Step Scoring method proposed by (Taylor, 1977) was chosen for two main reasons, it presents results in the literature with decent precision (Tsagkari, et al., 2015) (Gerrard, 2001), and also for the possibility of integrating it into mass and energy balances so process parameters such as reaction concentrations could also change the capital investment estimation. However, care should be advised in using such methods, in the biobutanol case, the biomass intake/capital investment ratio obtained was of around 1 for Scenario A and around 1.8 for Scenario B, the technical economic evaluations for second generation ethanol and butanol processes found in the literature yield much higher ratios, from 2.5 to 4.5 (Dias, et al., 2011) (Mariano, et al., 2013) (Mariano, et al., 2013) (Treasure, et al., 2014) (Gnansounou, et al., 2010) (Wright, et al., 2007). One factor to take into consideration when analyzing these numbers is that in this work investment refers solely to a second generation butanol plant, whereas in the literature researched capital investment refers also to the combined heat and power and in some cases the first generation ethanol production, also, capital investment varies if the project being evaluated is for a first plant of the technology or a Nth plant. Nevertheless, in his work Tsagkari also highlighted the risks of using such methods and pointed that they were mainly developed for petrochemical plants. The fact that the capex accuracy presents an important correlation to the economic results of the processes indicates that from the beginning of project development, care should be taken about technical decisions in regard of future impacts in capital costs.

In the three cases studied, different levels of process information were available. For the case of the biobutanol there is abundant information available in the literature for process information whereas for the muconic acid case all information came from a single patent and parts of the process had to be designed using rules of thumb such as crystallization and drying processes, resulting in a low detail mass and energy balance, and a low detail flowsheet. The different levels of information available did not hinder the risk analysis, as shown both in the biobutanol case as in the muconic acid case, suggesting that it is a method useful for early stage projects, and the results also suggested that such an analysis can provide relevant information for decision making process.

8. CHAPTER 8: SUGGESTIONS FOR NEXT STUDIES

8.1. Including Life Cycle Assessment in Risk Analysis;

Due to increasing awareness of the environmental impacts of the industry among the population and the also increasing concern that the activities of such industries might be endangering the environment, impact assessment of the manufacturing processes have grown to be an important part of project evaluation.

A life cycle analysis could be coupled to risk analysis in the same way as the economic analysis, probability distributions of the impacts and sensitivity on which aspects of the project influence the most the environmental impacts would be an important aid in project decisions.

8.2. Developing a Quick Capital Estimation Method for Biotechnological Processes

An important addition to the methodology of early stage risk analysis of biorefineries would be a capital estimation method that is calibrated specifically for biorefineries and biotechnological processes.

As observed in this work, the method used for quick capital estimation was able to yield capital investment results in a practical way, but its results should be seen with skepticism. The reason is that all the capital estimation methodologies developed so far were done for petrochemical plants, for instance, the method proposed by Taylor (Taylor, 1977), was developed with data from the construction of several plants belonging to the company ICI, the result is that these methods do not take into account the specificities of the biotechnological processes.

9. BIBLIOGRAPHY

Albarelli, J. 2013. *Produção de Açúcar e Etanol de Primeira e Segunda Geração: Simulação, Integração Energética e Análise Econômica.* Campinas : UNICAMP, 2013.

AliceWeb. 2015. Trade Data - Imports. *AliceWeb2.* [Online] Ministério do Desenvolvimento Indústria e Comércio, 2015. [Citado em: 27 de 11 de 2015.] aliceweb.desenvolvimento.gov.br/.

BASF. 2008. *n-Butanol.* 2008.

Batista, F. 2008. *Estudo do Processo de Destilação Alcoólica Contínua: Simulação de Plantas Industriais de Produção de Álcool Hidratado, Álcool Neutro e Cachaça.* Campinas : UNICAMP, 2008.

Bereche, R. 2011. *Modelagem e Integração Energética do Processo de Produção de Etanol a Partir da Biomassa de Cana-de-Açúcar.* Campinas : UNICAMP, 2011.

Bozell, J e Petersen, G. 2010. Technology Development for the Production of Biobased Products from Biorefinery Carbohydrates - the US Department of Energy's "Top 10" Revisited. *Green Chemistry.* 4, 2010, Vol. 12.

Bransby, D. 2008. Synchronization of Biofeedstocks and Conversion Technologies: Current Status and Future Prospects. [A. do livro] S Slack e M Wicks. *Reshaping American Agriculture to Meet its Biofuel and Biopolymer Roles.* Wooster : Ohio State University, 2008.

Brasil Econômico. 2014. *Presidente da Unica diz que setor está na UTI.* [Jornal Brasil Econômico] 2014.

Bray, K. 2007. OSBL Tips for Process Engineers. *Kansas City Chapter Technical Letter.* 2007, 5.

Brekke, K. 2007. Butanol, an Energy Alternative? *Ethanol Today.* 2007.

Bureau of Labor Statistics. 2013. bls.gov. *Bureau of Labor Statistics.* [Online] 2013. blz.gov/ils.

Carvalho, S. 2007. A Produção de Álcool: Do Proálcool ao Contexto Atual. *Congresso da Sociedade Brasileira de Economia, Administração e Sociologia Rural.* 45, 2007.

CEPEA. 2015. cepea.esalq.uso.br. *CEPEA.* [Online] USP, 2015. [Citado em: 27 de 11 de 2015.] http://cepea.esalq.usp.br/.

Chandel, A, Silva, S e Singh, O. 2012. Detoxification of Lignocellulose Hydrolysates: Biochemical and Metabolic Engineering Toward White Biotechnology. *Bioenergy Resources.* 2012.

Conab. 2008. *Perfil do Setor do Açúcar e do Álcool no Brasil.* Brasília : Companhia Nacional de Abastecimento, 2008.

Damodaran, A. 2006. *Probabilistic Approaches: Scenario Analysis, Decision Trees and Simulations.* 2006.

Dias, M, et al. 2011. Simulation of Integrated First and Second Generation Bioethanol Production from Sugarcane: Comparison Between Different Biomass Pretreatment Methods. *Journal of Industrial Microbiology Biotechnology.* 2011, 38.

Economist. 2015. Economist.com. *The Economist.* [Online] 18 de 04 de 2015. [Citado em: 06 de 01 de 2016.] http://www.economist.com/node/21648630/print.

Ely, R. 2009. *Avaliação Prospectiva das Rotas de Bio-Refinaria no Brasil, a Partir do Bagaço de Cana-de-Açúcar como Matéria-Prima Básica.* Rio de Janeiro : UFRJ/COPPE, 2009.

Embrapa. 2011. *Biorrefinarias: Cenários e Perspectivas.* Brasilia : Embrapa Agroenergia, 2011.

Ensinas, A. 2008. *Integração Térmica e Otimização Termoeconômica Aplicadas ao Processo Industrial de Produção de Açúcar e Etanol a Partir da Cana-de-Açúcar.* Campinas : UNICAMP, 2008.

Gerrard, A.M. 2001. *Guide to Capital Cost Estimating.* Warwickshire : IChemE, 2001.

Gnansounou, E e Dauriat, A. 2010. Techno-economic Analysis of Lignocellulosic Ethanol: A Review. *Bioresource Technology.* 2010, Vol. 101, 13.

Graham, P. 2012. Startup = Growth. *paulgraham.com.* [Online] 09 de 2012. [Citado em: 2 de 2 de 2015.] http://www.paulgraham.com/growth.html.

Green, E.M. 2011. Fermentative Production of Butanol - The Insdustrial Perspective. *Current Opinion in Biotechnology.* 2011, Vol. 22.

Hertz, D e Thomas, H. 1983. *Risk Analysis and its Applications.* Chichester : John Wyley and Sons, 1983.

Hertz, D. 1979. Risk Analysis in Capital Investment. *Harvard Business Review.* September - October 1979, 1979.

Hÿtonen, E and Stuart, P. 2012. Technoeconomic Assessment and Risk Analysis of Biorefinery Processes. [book auth.] M El-Hawagi and P Stuart. *Integrated Biorefineries: Design, Analysis and Optimization.* s.l. : CRC Press, 2012.

Hÿtonen, E and Stuart, P. 2009. Biofuel Production in an Integrated Forest Biorefinery - Technology Identification Under Uncertainties. *International Biorefinery Conference.* 2009.

ICIS. 2011. Icis.com. *ICIS.* [Online] 05 de 12 de 2011. [Citado em: 05 de 08 de 2015.] http://www.icis.com/resources/news/2011/12/05/9513406/green-chemicals-growing-number-of-chemical-firms-enter-bio-butanol-space/.

Klein-Marcushamer, D, et al. 2011. The Challenge of Enzyme Cost in the Production of Lignocellulosic Biofuels. *Biotechnology and Bioengineering.* 2011, Vol. 109.

Lanzotti, C. 2000. *Uma Análise Emergética de Tendências do Setor Sucroalcooleiro.* Campinas : UNICAMP, 2000.

Mansur, M, et al. 2010. *ABE Fermentation of Sugar in Brazil.* Philadelphia : University of Pennsylvania, 2010.

Mariano, A. P., et al. 2013. Utilization of Pentoses from Sugarcane Biomass: Techno-economics of Biogas vs Butanol Production. *Bioresource Technology.* 2013, 142.

Mariano, A.P, et al. 2013. Butanol Production in a First-Generation Brazilian Sugarcane Biorefinery: Technical Aspects and Economics of Greenfield Projects. *Biresource Technology.* 2013, Vol. 135.

Martins, F e Gay, J. 2014. *Biofuels: From Boom to Bust?* São Paulo : Bain & Company, 2014.

Myriant. 2013. *Production of Muconic Acid from Geneticaly Engineered Microorganisms. CA 2862051* Canada, 08 de 08 de 2013.

NREL. 2004. *Top Added Value Chemicals from Biomass Volume I: Results of Screening for Potential Candidates from Sugars and Synthesis Gas.* Oak Ridge : NREL, 2004.

Oliveira, A. 2010. *Análise Prospectiva da Utilização de uma Usina como Plataforma para uma Biorrefinaria.* São Paulo : FGV, 2010.

Peters, M e Timmerhaus, K. 1991. *Plant Design and Economics for Chemical Engineers.* s.l. : McGraw Hill, 1991.

Petley, G. 1997. *A Method for Estimating the Capital Cost of Chemical Process Plants: Fuzzy Matching.* s.l. : Loughborough University, 1997.

Petrobras. 2015. petrobras.com.br. *Petrobras.* [Online] Petrobras, 26 de 12 de 2015. [Citado em: 06 de 01 de 2016.] http://www.petrobras.com.br/pt/produtos-e-servicos/composicao-de-precos/gasolina/.

Ree, R e Annevelink, B. 2007. *Status Report Biorefinery 2007.* Wageningen : Agrotechnology and Food Sciences Group, 2007.

Rein, P. 2007. *Cane Sugar Engineering.* Berlin : Bartens, 2007.

Robehmed, N. 2013. What is a Startup. *Forbes.com.* [Online] 16 de 12 de 2013. [Citado em: 2 de 2 de 2015.] http://www.forbes.com/sites/natalierobehmed/2013/12/16/whatisastartup/.

Rodrigues, A. 2012. Etanol e o Setor Sucroenergético: Situação Atual e Perspectivas. Brasília : Unica, 2012.

Sengupta, D. 2010. *Integrating Bioprocesses Into Industrial Complexes for Sustainable Deveopment.* s.l. : Louisiana State University, 2010.

Taylor, J. 1977. The 'Process Step Scoring' Method for Making Quick Capital Estimates. *Engineering and Process Economics.* 1977, Vol. 2.

Treasure, T, et al. 2014. Integrated Conversion, Financial, and Risk Modeling of Cellulosic, Ethanol from Woody and non-Woody Biomass via Dilute Acid Pretreatment. *Biofuels, Bioproducts & Biorefining.* 2014, 8.

Tsagkari, M, et al. 2015. Heuristics for Capital Cost Estimation: A Case Study of Biorefinery Processes. *National Congress of Chemical Engineering.* 2015, 10.

Turton, R, et al. 2012. *Analysis, Synthesis and Design of Chemical Processes.* New York : Prentice Hall, 2012.

van der Merwe, A. 2010. *Evaluation of Different Process Designs for Biobutanol Production from Sugarcane Molasses.* Stellenbosh : University of Stellenbosh, 2010.

Wright, M e Brown, R. 2007. Comparative Economics of Biorefineries Based on the Biochemical and Thermochemical Platforms. *Biofuels, Bioproducts & Biorefining.* 2007, Vol. 1.

Xinxiao, S, et al. 2013. A Novel Muconic Acid Biosynthesis Approach by Shunting Tryptophan Biosynthesis via Anthranilate. *Applied and Environmental Microbiology.* 2013, Vol. 79, 13.